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Interactions in flavanone and chalcone derivatives: Hirshfeld surface analysis, energy frameworks and global reactivity descriptors

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The present study examines a series of flavanone and chalcone derivatives substituted with electron-withdrawing groups (Cl or Br) and electron-donating groups (OH, CH_3 and OCH_3), namely, 7-methoxy-2-phenyl-3,4-dihydro-2*H*-1-benzopyran-4-one, $C_{16}H_{14}O_3$, 2-(4-methoxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-4-one, $C_{16}H_{14}O_3$, 2-(4-methoxyphenyl)-6-methyl-3,4-dihydro-2*H*-1-benzopyran-4-one, $C_{17}H_{16}O_3$, 2-(4-chlorophenyl)-3,4-dihydro-2*H*-1-benzopyran-4-one, $C_{15}H_{11}ClO_2$, 8-bromo-6-methyl-2-phenyl-3,4-dihydro-2*H*-1-benzopyran-4-one, $C_{16}H_{13}BrO_2$, (2*E*)-1-(2-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one, $C_{16}H_{14}O_3$, and (2*E*)-1-(2-hydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one, $C_{15}H_{12}O_3$. It compares the two groups of derivatives with regard to their intermolecular interactions in the crystal lattice and lattice energy calculations, together with energy framework visualization and global reactivity descriptors (chemical hardness, chemical potential and electrophilicity index). It also discusses the relationships between different noncovalent interactions derived from Hirshfeld surface analysis, crystal lattice energy and global reactivity descriptors of the compounds.

1. Introduction

The flavonoids, a group of polyphenolic compounds, constitute one of the most important families of natural products. As secondary metabolites of plants, they perform a range of functions, including pigmentation, a natural defence against pathogenic microorganisms and herbivores, and serve to protect the plant against UV-light exposure (Bonetti *et al.*, 2017). Flavonoids are found in edible plants and in a large number of foods of plant origin. Among the flavonoids, the chalcone (**CH**) and flavanone (**FL**) classes have attracted much attention due to their wide-ranging antioxidant (Hsiao *et al.*, 2007), antibacterial (Xu *et al.*, 2019; Dan & Dai, 2020) and cancer-preventive potential (Szliszka *et al.*, 2012), as well as their neuroprotective and hepatoprotective effects (Karimi-Sales *et al.*, 2018; Mahapatra *et al.*, 2015). Chalcones and their derivatives are incorporated in a wide range of synthetic applications and possess multitarget broad-spectrum biological activity (Zhuang *et al.*, 2017). A vast number of naturally occurring flavanones and chalcones demonstrate polyhydroxylation in their aryl rings. New potentially bioactive chalcone- and flavanone-like molecules have been synthesized by the incorporation of different functionalities in both rings (Scheme 1) (Rosa *et al.*, 2017).

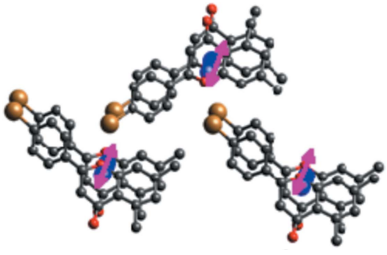


Table 1
Experimental details.

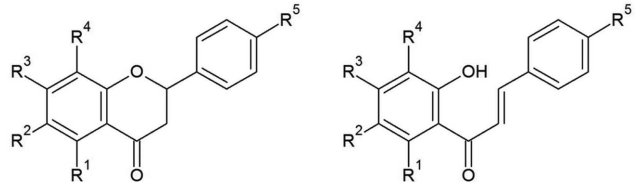
Experiments were carried out at 100 K with Mo $K\alpha$ radiation. Absorption was corrected for by multi-scan methods (*CrysAlis PRO*; Rigaku OD, 2015). H-atom parameters were constrained.

	FL1	**FL2**	**FL3**	**FL5**
Crystal data				
Chemical formula	$C_{16}H_{14}O_3$	$C_{16}H_{14}O_3$	$C_{17}H_{16}O_3$	$C_{15}H_{11}ClO_2$
M_r	254.27	254.27	268.30	258.69
Crystal system, space group	Monoclinic, $P2_1/c$	Orthorhombic, $Pbcn$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$
a, b, c (Å)	8.5168 (3), 6.6031 (2), 23.3468 (7)	12.7692 (2), 8.5258 (1), 23.1820 (3)	16.7561 (3), 8.0448 (1), 21.3319 (4)	6.4760 (2), 16.2902 (4), 11.6755 (4)
α, β, γ (°)	90, 90.737 (3), 90	90, 90, 90	90, 110.138 (2), 90	90, 97.953 (3), 90
V (Å^3)	1312.85 (7)	2523.77 (6)	2699.74 (8)	1219.86 (6)
Z	4	8	8	4
μ (mm^{-1})	0.09	0.09	0.09	0.30
Crystal size (mm)	0.3 × 0.2 × 0.1	0.4 × 0.2 × 0.1	0.3 × 0.2 × 0.1	0.3 × 0.2 × 0.1
Data collection				
Diffractometer	Agilent SuperNova Dual Source diffractometer with an Atlas detector	Agilent SuperNova Dual Source diffractometer with an Atlas detector	Agilent SuperNova Dual Source diffractometer with an Atlas detector	Agilent SuperNova Dual Source diffractometer with an Atlas detector
T_{min}, T_{max}	0.341, 1.000	0.671, 1.000	0.752, 1.000	0.801, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20587, 2724, 2550	19929, 2615, 2267	21035, 5586, 4898	16927, 2525, 2414
R_{int}	0.025	0.027	0.024	0.015
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.628	0.628	0.628	0.628
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.112, 1.05	0.056, 0.144, 1.04	0.044, 0.108, 1.04	0.027, 0.073, 1.06
No. of reflections	2724	2615	5586	2525
No. of parameters	183	183	391	163
No. of restraints	0	3	5	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.40, −0.34	0.46, −0.53	0.40, −0.32	0.32, −0.26

	FL8	**CH2**	**CH4**
Crystal data			
Chemical formula	$C_{16}H_{13}BrO_2$	$C_{16}H_{14}O_3$	$C_{15}H_{12}O_3$
M_r	317.17	254.29	240.26
Crystal system, space group	Monoclinic, $P2_1/n$	Orthorhombic, $Pca2_1$	Monoclinic, $P2_1$
a, b, c (Å)	15.2121 (7), 8.7614 (2), 20.7260 (6)	25.297 (2), 4.0469 (2), 12.6390 (16)	3.9413 (2), 17.3664 (8), 17.2360 (9)
α, β, γ (°)	90, 92.458 (3), 90	90, 90, 90	90, 94.504 (5), 90
V (Å^3)	2759.81 (16)	1293.9 (2)	1176.10 (10)
Z	8	4	4
μ (mm^{-1})	2.97	0.09	0.09
Crystal size (mm)	0.2 × 0.1 × 0.1	0.40 × 0.18 × 0.08	0.50 × 0.08 × 0.06
Data collection			
Diffractometer	Agilent SuperNova Dual Source diffractometer with an Atlas detector	Rigaku Xcalibur with a Sapphire3 detector	Rigaku Xcalibur with a Sapphire3 detector
T_{min}, T_{max}	0.524, 1.000	0.876, 1.000	0.758, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30046, 5682, 4561	12934, 3120, 3037	9466, 4835, 4459
R_{int}	0.051	0.022	0.021
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.628	0.661	0.628
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.095, 1.05	0.028, 0.078, 1.05	0.030, 0.073, 1.04
No. of reflections	5682	3120	4835
No. of parameters	351	174	329
No. of restraints	6	1	1
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.98, −0.61	0.24, −0.14	0.15, −0.17
Absolute structure	–	Flack x determined using 1419 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 1981 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	–	−0.4 (3)	−0.2 (5)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *publCIF* (Westrip, 2010).

Chalcones are key precursors in the biosynthesis of flavanones and other flavonoids. In plants, the synthesis of chalcone from malonyl–CoA (CoA is coenzyme A) and *p*-coumaroyl–CoA, catalysed by chalcone synthase, is followed by their intramolecular and stereospecific cyclization into (2*S*)-flavanone. Chalcone isomerases are specific for the formation of the six-membered heterocyclic ring characteristic of flavanones. Two such isomers, *i.e.* *ortho*-hydroxychalcone and flavanone, can undergo reversible isomerization in solution (Mai *et al.*, 2013); this *ortho*-hydroxychalcone/flavanone pair is a good example of molecular switching, where molecules are capable of predictable and reversible conformational changes. Such compounds have become increasingly desirable targets for organic synthesis (Mai *et al.*, 2013; Muller *et al.*, 2016). Moreover, the physicochemical properties of chalcone and its derivatives, including their nonlinear optical and fluorescence properties, have received considerable attention owing to their associated delocalization of electronic charge distribution and overlapping π-orbitals. Furthermore, the optical properties are related not only to the particular molecule, but are also heavily dependent on the crystal structure and intermolecular packing. It is therefore beneficial to determine the packing of the crystal structure by a detailed analysis of the intermolecular contacts. In addition, by introducing electron donor or acceptor groups to the aromatic rings of the chalcone scaffold, it is possible to modulate their optical properties and obtain chalcone derivatives with strong fluorescence, both in solution and in the solid state. The aim of this study is to provide comprehensive structural information for a series of 15 compounds, both flavanones and chalcones. Three aspects of these compounds are evaluated: (i) intermolecular interactions in the crystal lattice using the Hirshfeld surface approach (Spackman & Jayatilaka, 2009), (ii) lattice energy analysis (Turner *et al.*, 2014), including energy framework visualization (Turner *et al.*, 2015), and (iii) electronic molecular properties based on density functional theory (DFT) global reactivity descriptors. Seven compounds (five flavanones and two chalcones), namely, 7-methoxy-2-phenyl-3,4-dihydro-2*H*-1-benzopyran-4-one, **FL1**, 2-(4-methoxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-4-one, **FL2**, 2-(4-methoxyphenyl)-6-methyl-3,4-dihydro-2*H*-1-benzopyran-4-one, **FL3**, 2-(4-chlorophenyl)-3,4-dihydro-2*H*-1-benzopyran-4-one, **FL5**, 8-bromo-6-methyl-2-phenyl-3,4-dihydro-2*H*-1-benzopyran-4-one, **FL8**, (2*E*)-1-(2-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one, **CH2**, and (2*E*)-1-(2-hydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one, **CH4**, were obtained as single crystals and their structures were solved and refined using X-ray diffraction data. As flavanones and chalcones are isomers of each other, it is possible to identify structural similarities and differences between them in terms of their weak intermolecular interactions in the crystal lattice and their energetics. To form an isomer pair with the self-solved structure, the appropriate compound was searched for in the Cambridge Structural Database (CSD, Version 5.39, 2018 release; Groom *et al.*, 2016). Based on the results of the CSD search, two flavanone–chalcone pairs were added, thus increasing the total number of halogen-substituted compounds. Finally, the number of compounds was expanded to include the following: **CH1** (Serdiuk *et al.*, 2018; CSD refcode REPXIW), **CH3** (Fun *et al.*, 2011; URESOA), **FL4** (Białońska *et al.*, 2007; NUYRII01), **CH5** (Fun *et al.*, 2007; QEXLAH), **FL6** (Cantrell *et al.*, 1974; BRFLAY20), **CH6*A*/*B*** [two different polymorphs; Agilandeshwari *et al.* (2016) (IKOFAR); Salinas-Ortega *et al.* (2017) (IKOFAR01)], **FL7** (Goud *et al.*, 1995; YIVREA) and **CH7** (Goud *et al.*, 1995; YIVPUO) (Scheme 1). Unfortunately, in the case of flavanone **FL8**, the corresponding CIF is not present in the CSD.



Code	R^1	R^2	R^3	R^4	R^5
FL1, CH1	H	H	OCH_3	H	H
FL2, CH2	H	H	H	H	OCH_3
FL3, CH3	H	CH_3	H	H	OCH_3
FL4, CH4	H	H	H	H	OH
FL5, CH5	H	H	H	H	Cl
FL6, CH6	H	H	H	H	Br
FL7, CH7	CH_3	H	CH_3	H	Br
FL8	H	CH_3	H	Br	H

Scheme 1

2. Experimental

2.1. X-ray diffraction

All H atoms were fixed geometrically at calculated positions using a riding model. The structures of **FL3**, **FL8** and **CH4** crystallize with two molecules in the asymmetric unit. In four refined structures, one or two C atoms of the heterocyclic ring were found to be disordered and were refined with two alternative positions, *A* and *B* (atom name, final site-occupancy factors for major component *A*), for **FL1** [C2 atom, k_A = 0.533 (6)], **FL2** [C2 atom, k_A = 0.526 (7)], **FL3** [C2 and C3 atoms, k_A = 0.549 (7); C52 and C53 atoms, k_A = 0.932 (3)] and **FL8** [C2 atom, k_A = 0.928 (7); C52 atom, k_A = 0.814 (7)]. Table 1 reports the results of the crystal structure determinations.

2.2. Model energy calculations and Hirshfeld surface analysis

The crystal structure geometries of the studied compounds were subsequently used to calculate interaction energies using *CrystalExplorer17* (Turner *et al.*, 2017; Mackenzie *et al.*, 2017) and *GAUSSIAN09* (Frisch *et al.*, 2013). Accurate pairwise model energies, based on the B3LYP/6-31G(d,p) molecular wave function, were estimated between any nearest-neighbour molecular pairs within a cluster of 20 Å for dipolar molecules and 25 Å for nondipolar molecules. The energy framework was constructed based on the total interaction energy, esti-

Table 2
Ring puckering parameters with asymmetry parameters and the dihedral angle between the chromone skeleton (*A*/*B* rings) and ring *C*.

Compound	*Q* (Å)	θ (°)	Φ (°)	Asymmetry parameters (°)	Conformation	Dihedral angle *A*/*B* skeleton and *C* ring (°)
FL1	0.330 (2)	129.3 (3)	237.7 (4)	ΔCs(C2*A*) = 2.8 (2)	E	89.2 (2)
FL2	0.340 (3)	128.7 (3)	248.5 (4)	ΔCs(C2*A*) = 4.4 (2)	E	74.7 (2)
FL3_*A*	0.505 (3)	127.8 (3)	273.2 (3)	ΔC2(C2*A*—C3*A*) = 3.1 (3)	S/B	53.2 (2)
FL3_*B*	0.522 (2)	119.85 (18)	243.19 (14)	ΔCs(C52*A*) = 1.3 (2)	E	67.9 (2)
FL5	0.511 (2)	118.94 (13)	243.79 (14)	ΔCs(C2) = 1.8 (2)	E	74.3 (2)
FL8_*A*	0.474 (4)	54.6 (5)	82.0 (5)	ΔC2(C2*A*—C3) = 9.4 (4)	B, T/B	46.3 (2)
FL8_*B*	0.456 (4)	58.5 (5)	61.7 (5)	ΔCs(C52*A*) = 0.4 (4)	E	77.7 (2)

Notes: the *Q*, θ and Φ puckering parameters were calculated according to Cremer & Pople (1975); ΔCs and ΔC2 are asymmetry parameters calculated according to Duax & Norton (1975); E, B, S/B and T/B define the conformations envelope, boat, between screw-boat and boat, and between twist boat & boat, respectively. FL3/8_*A*/*B* corresponds to two different molecules in the asymmetric unit.

mated in terms of four components, *viz.* electrostatic, polarization, dispersion and exchange–repulsion, with scale factors of 1.057, 0.740, 0.871 and 0.618, respectively. In the present study, the positional parameters of the major component (*A*) were chosen for the coordinates of the disordered atoms. According to *CrystalExplorer* procedures, the bond lengths to H atoms were normalized to standard neutron values. *CrystalExplorer17* (Turner *et al.*, 2017; Mackenzie *et al.*, 2017) was also used to generate the Hirshfeld surface (Spackman & Jayatilaka, 2009; McKinnon *et al.*, 1998).

2.3. Calculation of lattice energies

The CE-B3LYP lattice energies were calculated according to Thomas *et al.* (2018) as half of the direct summation gained by the multiplication of E_{tot} and N, where N is the number of molecule pairs in the cluster with that particular interaction energy for the nonpolar space group.

$$E_{lat}^{CE-B3LYP} = 0.5 \sum_{R_{AB}<R} E_{tot}^{AB} \quad (1)$$

However, the polar space group ($Pca2_1$ for **CH2** and $P2_1$ for **CH4**, **CH6*A*** and **FL7**) needs special consideration and the lattice energy is:

$$E_{lat}^{CE-B3LYP} = 0.5 \sum_{R_{AB}<R} E_{tot}^{AB} + E_{cell\ dipole}$$

$$= 0.5 \sum_{R_{AB}<R} E_{tot}^{AB} - \frac{2\pi p_{cell}^2}{3VZ_{cell}} \quad (2)$$

In equation (2), the second term is a correction of the cell dipole, where p_{cell} is a magnitude of the cell dipole moment, obtained as the sum of the vectors of the molecular dipole moments; V_{cell} and Z_{cell} represent the volume and number of unique molecules in the unit cell.

2.4. Calculations of global reactivity descriptors

The energies of frontier molecular orbitals, namely, the lowest unoccupied molecular orbital (E_{LUMO}) and the highest occupied molecular orbital (E_{HOMO}), were calculated based on the CIF files. First, each CIF was opened in *CrystalExplorer* and, after normalization of the C—H and O—H bond lengths to 1.083 and 0.983 Å, respectively, the input file for *GAUSSIAN09* was generated. The energies of the two orbitals were calculated using the B3LYP/6-31G(d,p) basis set. The HOMO and LUMO orbital energies were used to evaluate the following global reactivity descriptors: chemical potential [$\mu = (E_{LUMO} + E_{HOMO})/2$], chemical hardness [$\eta = (E_{LUMO} - E_{HOMO})/2$], softness ($\sigma = 1 - \eta$) and electrophilicity ($\omega = \mu^2/2\eta$). All computed values of the electron structure descriptors are summarized in Table S5 of the supporting information.

3. Results and discussion

3.1. Structural commentary

The molecular structures of **FL1**, **FL2**, **FL3**, **FL5**, **FL8**, **CH2** and **CH4** are shown in Figs. 1–7. The main body of the flavanone structure consists of two fused rings, namely, a benzene ring and a pyran ring, with a phenyl ring substituted at atom C2 with different substituents at the *para* positions. The pyran rings adopt mainly envelope (E) or screw-boat (S) conformations with small asymmetry parameters (Duax & Norton, 1975) (Table 2); however, one molecule of **FL8** displays a pyran ring demonstrating a conformation between boat and twist-boat. The appropriate puckering parameters (Cremer & Pople, 1975) are presented in Table 2. Although the geometric parameters for the chromanone skeleton do not differ signif-

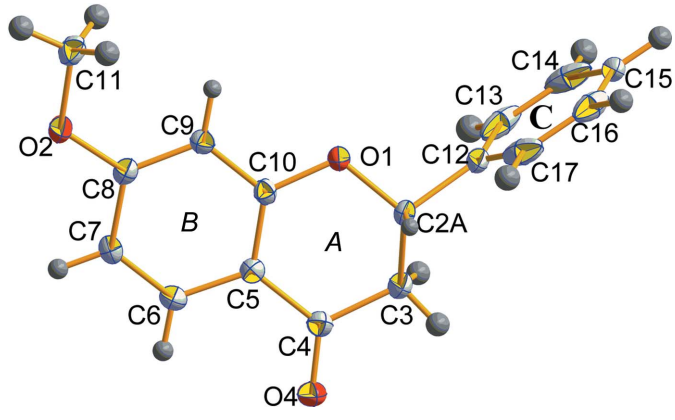


Figure 1
A view of the molecular structure of **FL1**, showing the atom-numbering scheme. Displacement parameters are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius.

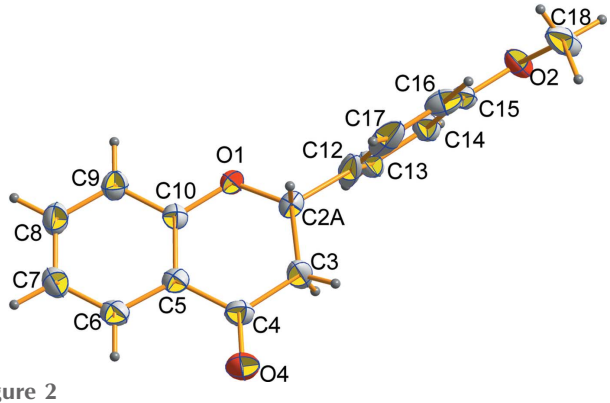


Figure 2
A view of the molecular structure of **FL2**, showing the atom-numbering scheme. Displacement parameters are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius.

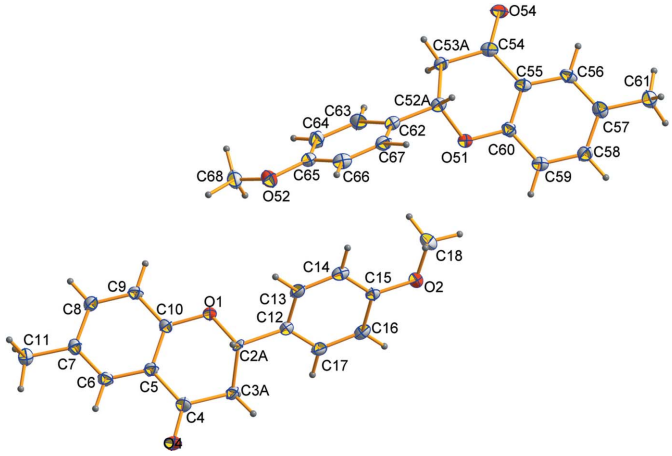


Figure 3
A view of the two independent molecules of the structure of **FL3**, showing the atom-numbering scheme. Displacement parameters are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius.

icantly, the phenyl ring substituted at the C2 atom is usually inclined at an angle between 46.3 (2) and 89.2 (2)° with respect to the main skeleton (Fig. 8), as reflected in the dihedral angles between rings *A*/*B* and *C* (Table 2). As expected, the main

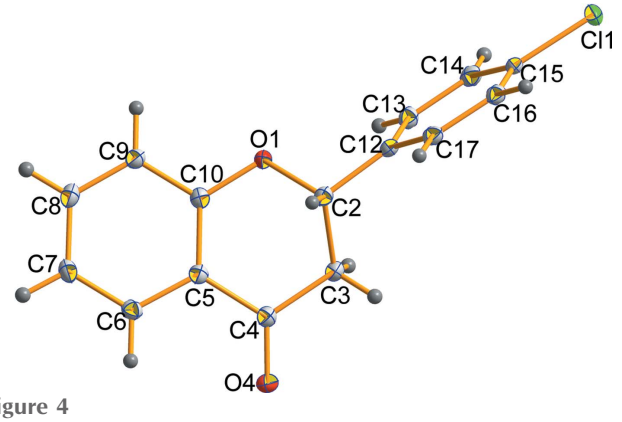


Figure 4
A view of the molecular structure of **FL5**, showing the atom-numbering scheme. Displacement parameters are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius.

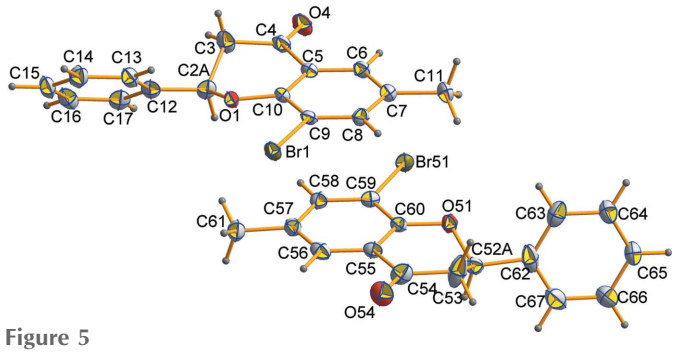


Figure 5
A view the two independent molecules of the structure **FL8**, showing the atom-numbering scheme. Displacement parameters are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius.

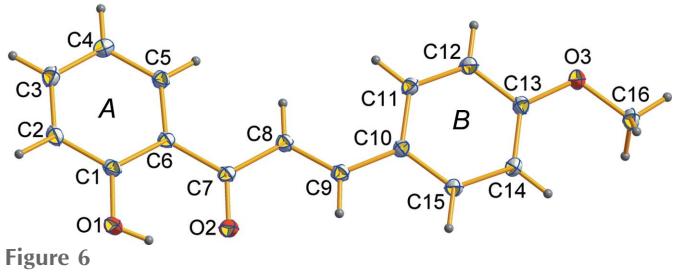


Figure 6
A view the two independent molecules of the structure of **CH2**, showing the atom-numbering scheme. Displacement parameters are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius.

body of the chalcone structure consists of two nearly coplanar six-membered aromatic rings (*A* and *B*) connected by a three-carbon α,β-unsaturated chain with a planar configuration along the double C=C bond. The appropriate torsion angle for the **CH2** molecule is C6—C7—C8—C9 of 178.5 (2)°; for

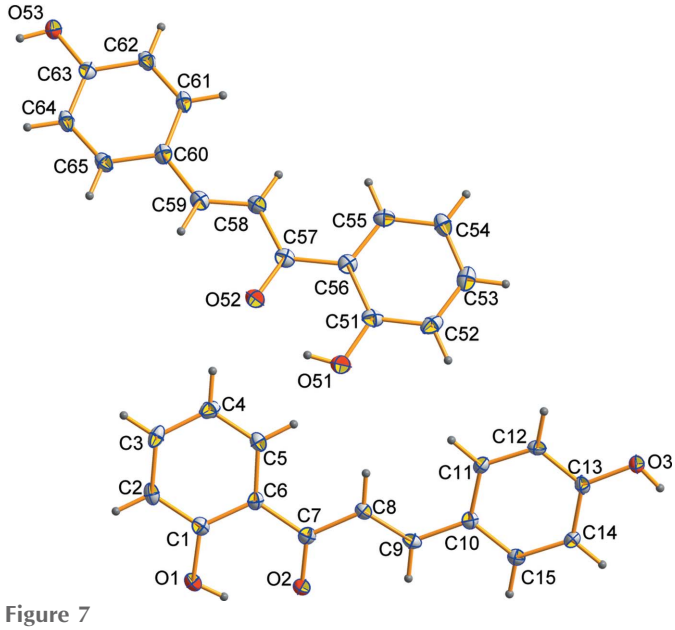


Figure 7
A view the two independent molecules of the structure of **CH4**, showing the atom-numbering scheme. Displacement parameters are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius.

Table 3
Hydrogen-bond geometry (Å, °) for **FL1**.

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···O4^{i}	0.95	2.64	3.439 (3)	158

Symmetry code: (i) $x+1, y-1, z$.

Table 4
Hydrogen-bond geometry (Å, °) for **FL2**.

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O4^{i}	0.95	2.51	3.365 (3)	149
C2A—H2A···O4^{ii}	1.00	2.21	3.150 (3)	156

Symmetry codes: (i) $x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, z$.

Table 5
Hydrogen-bond geometry (Å, °) for **FL3**.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O4^{i}	0.95	2.55	3.231 (2)	129
C16—H16···O1^{ii}	0.95	2.51	3.415 (2)	160
C52A—H52A···O54^{iii}	1.00	2.35	3.216 (2)	145
C68—H68B···O4^{iv}	0.98	2.46	3.330 (2)	147

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+2, -y+1, -z+1$.

Table 6
Hydrogen-bond geometry (Å, °) for **FL5**.

D—H···A	D—H	H···A	D···A	D—H···A
C15—Cl1···O4^{i}	1.75	3.05 (1)	4.798 (2)	175

Symmetry code: (i) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

CH4, the torsion angles are equal, with C6—C7—C8—C9 = 178.4 (2)° (molecule *A*) and C56—C57—C58—C59 = 179.2 (2)° (molecule *B*).

3.2. Supramolecular features

In the packing structure of **FL1**, the molecules are connected *via* a C15—H15···O4^{i} hydrogen bond [symmetry code: (i) $x+1, y-1, z$], forming chains along the [1$\bar{1}$0] direction with a $C(9)$ graph-set motif (Etter, 1990) (Table 3 and Fig. 9). The crystal packing of **FL1** is also dominated by C—H···π and π–π interactions (Tables S2 and S3 in the supporting information).

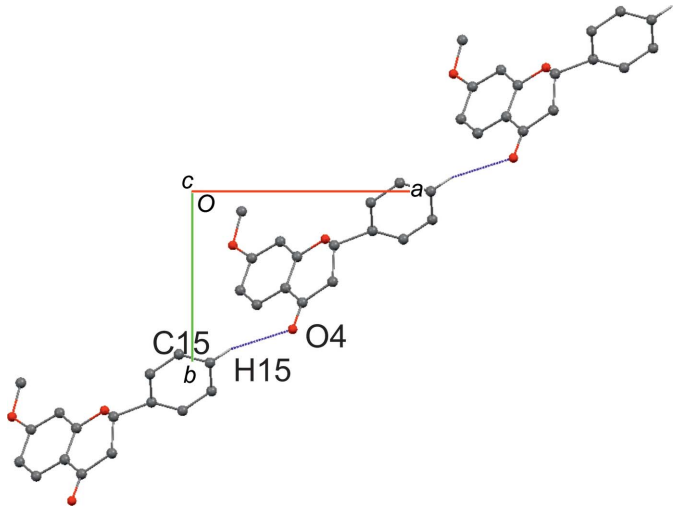
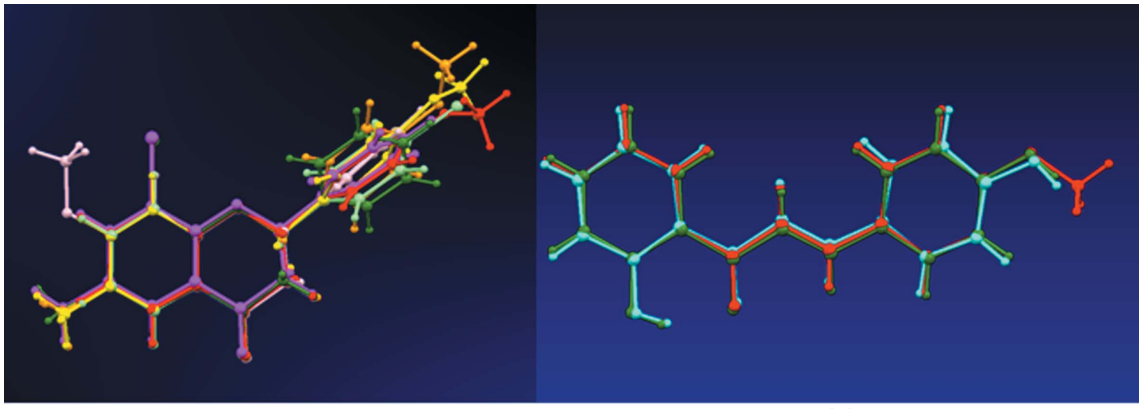


Figure 9
The crystal structure of **FL1**, with hydrogen bonds, showing chains along the [1$\bar{1}$0] direction.

The packing of **FL2** (Fig. 10) is dominated by C2A—H2A···O4^{i} and C16—H16···O4^{ii} intermolecular hydrogen bonds [symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$] (Table 4) and two C—H···π interactions (Table S2 in the supporting information). The C2A—H2A···O4^{ii} interaction links the molecules into chains that are parallel to the *b* axis and have the graph-set motif $C(6)$, while the C16—H16···O4^{i} interaction forms chains along the [110] direction with the graph-set notation $C(8)$ (Etter, 1990).

Compound **FL3** crystalizes in the space group $P2_1/n$ with two independent molecules in the asymmetric unit. Its crystal structure seems to be stabilized by a combination of C—H···O, C—H···π and π–π interactions (Table 5, and Tables S2 and S3 in the supporting information). The C8—H8···O4^{i} and C16—H16···O1^{ii} hydrogen bonds [symmetry codes: (i) $x, y-1, z$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$] form $C(7)$ and $C(6)$ chains parallel to the *b* axis (Fig. 11*a*). The combination of these interactions



(*a*) (*b*)

Figure 8
An overlay of (*a*) the flavanone and (*b*) the chalcone molecular structures. The colour code is: pink **FL1**, red **FL2**, orange/yellow **FL3*A*/*B***, light green **FL5**, green/magenta **FL8*A*/*B***, red **CH2** and green/cyan **CH4*A*/*B***.

Table 7
Hydrogen-bond geometry (Å, °) for **FL8**.

D—H···A	D—H	H···A	D···A	D—H···A
C2A—H2A···O54^{i}	1.00	2.57	3.396 (5)	140
C53—H53A···O4^{ii}	0.99	2.53	3.399 (5)	147

Symmetry codes: (i) $x, y+1, z$; (ii) $x, y-1, z$.

Table 8
Hydrogen-bond geometry (Å, °) for **CH2**.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	1.80	2.532 (2)	147
C5—H5···O1^{i}	0.93	2.53	3.364 (5)	150
C9—H9···O2	0.93	2.44	2.790 (2)	103

Symmetry code: (i) $-x+\frac{3}{2}, y, z-\frac{1}{2}$.

closes the rings described by the graph-set notation as $R_3^3(19)$ (Etter, 1990). The *B* molecules of **FL3** also interact with each other *via* the C52A—H52A···O54^{iii} hydrogen bond [symmetry code: (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$], propagating the $C(5)$ chain along the *b* axis (Fig. 11*b*) (Etter, 1990). The C68—H68B···O4^{iv} hydrogen bond [symmetry code: (iv) $-x+2, -y+1, -z+1$] acts as a linker between molecules *A* and *B* (Fig. 11*c*).

Table 9
Hydrogen-bond geometry (Å, °) for **CH4**.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	1.84	2.570 (2)	147
O3—H31···O2^{i}	0.82	1.96	2.783 (5)	176
O51—H51···O52	0.82	1.82	2.539 (2)	146
O53—H531···O3^{ii}	0.82	1.99	2.803 (2)	169
C4—H4···O52	0.93	2.57	3.356 (3)	143
C15—H15···O53^{iii}	0.93	2.53	3.404 (3)	156

Symmetry codes: (i) $-x+2, y-\frac{1}{2}, -z$; (ii) $-x+1, y+\frac{1}{2}, -z+1$; (iii) $x+1, y, z-1$.

In the crystal structure of **FL5**, the only hydrogen bonds which are observed belong to the C—H···π type (Table S2 in the supporting information). However, it seems that the

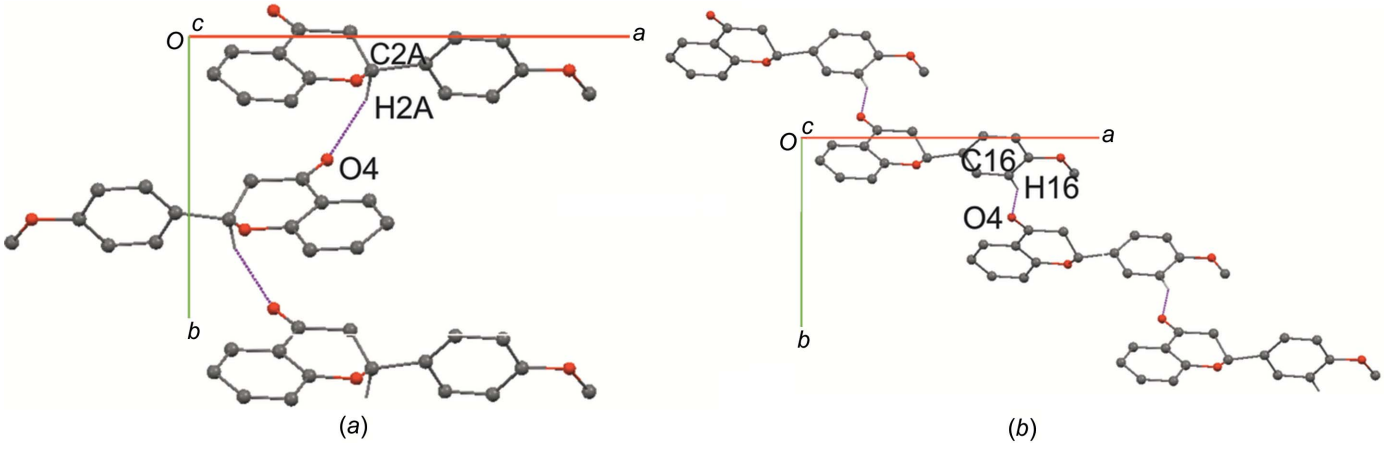


Figure 10
The crystal structure of **FL2**, with hydrogen bonds, showing (*a*) $C(6)$ chains along the *b* axis and (*b*) $C(8)$ chains along the [110] direction.

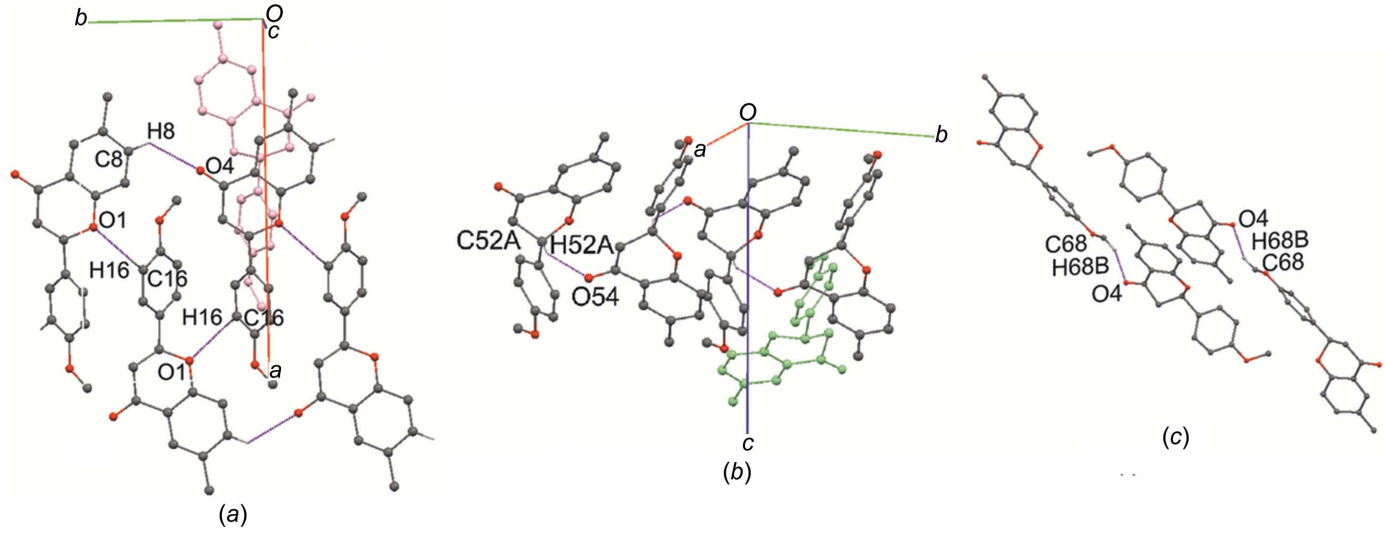


Figure 11
The crystal structure of **FL3**, with hydrogen bonds, showing (*a*) $C(7)$ and $C(6)$ chains of *A* molecules connected to ring $R_3^3(19)$ and (*b*) a $C(5)$ chain of *B* molecules along the *b* axis. (*c*) Two independent molecules linked by the C68—H68···O4^{iv} interaction. Green/pink molecules represent molecules *A*/*B*.

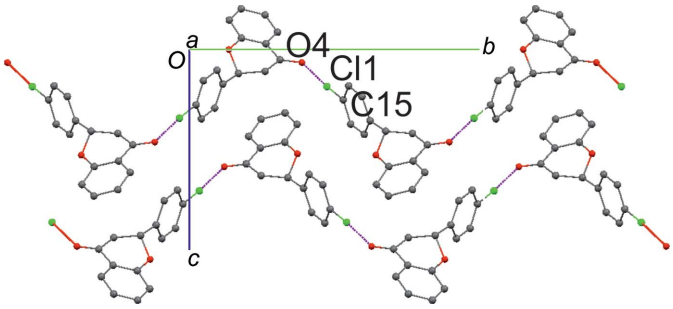


Figure 12
The formation of a zigzag chain along the *b* axis for the crystal structure of compound **FL5**.

crystal packing of **FL5** is mostly stabilized by the C15—Cl1···O4^{i} halogen bond [symmetry code: (i) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$], where molecules are linked into the zigzag $C(9)$ chain propagating along the *b* axis (Fig. 12 and Table 6) (Etter, 1990).

Similar to **FL3**, **FL8** crystallizes in the monoclinic space group $P2_1/n$, with two independent molecules in the asymmetric unit, which are self-assembled into dimers through the C2*A*—H2*A*···O54^{i} and C53—H53*A*···O4^{ii} hydrogen bonds [symmetry codes: (i) $x, y+1, z$; (ii) $x, y-1, z$] (Table 7). This motif can be described using graph-set notation as $R_2^2(8)$ (Fig. 13) (Etter, 1990). Furthermore, both C—H···π and π–π interactions are also evident in the crystal lattice (Tables S2 and S3 in the supporting information).

The crystal structure of chalcone **CH2** is dominated by the presence of C5—H5···O1^{i} hydrogen bonds [symmetry code: (i) $-x+\frac{3}{2}, y, z-\frac{1}{2}$], which connect molecules into a $C(5)$ chain propagating along the *c* axis (Fig. 14) (Etter, 1990). It is worth mentioning that the close proximity between donor atoms O1 and C9 and acceptor atom O2 allows two intramolecular hydrogen bonds to be formed (Table 8). In addition, in the crystal lattice, a short distance is observed between the O2 atom and π-electrons from ring *A* of the molecule related by the symmetry code ($x, y-1, z$) (Table S2 in the supporting information).

Compound **CH4** crystallizes in the monoclinic space group $P2_1$, with two independent molecules in an asymmetric unit.

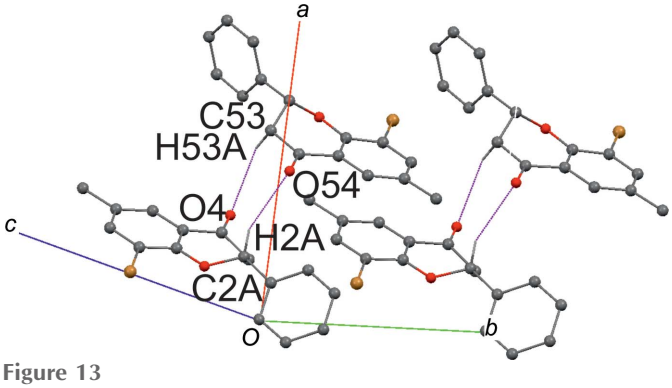


Figure 13
A fragment of the molecular structure of **FL8**, with rings formed between two independent molecules.

The geometries of these two molecules do not differ significantly from each other (Fig. 8). The crystal structure includes a combination of O—H···O, C—H···O and π–π interactions (Table 9). Atom O3 acts as a donor for the O3—H31···O2^{i} hydrogen bond [symmetry code: (i) $-x+2, y-\frac{1}{2}, -z$], forming a chain along the *b* axis between *A* molecules, while the O53—H53···O3^{ii} hydrogen bond [symmetry code: (ii) $-x+1, y+\frac{1}{2}, -z+1$] joins *B* molecules into the main chain, forming a structure reminiscent of a 'fir' tree (Fig. 15*a*). The C15—H15···O53^{iii} and C4—H4···O52 hydrogen bonds [symmetry code: (iii) $x+1, y, z-1$] link molecules *A* and *B* alternately, forming a chain parallel to the [$\bar{1}$01] direction (Fig. 15*b*) (Etter, 1990).

3.3. Hirshfeld surface analysis

The presence of all the noncovalent interactions involved in the crystal structure, *i.e.* O—H···O, C—H···O, C—H···π, π–π and C—H···Cl/Br, can be analysed and visualized by their Hirshfeld surfaces (HS) (Spackman & Byrom, 1997; McKinnon *et al.*, 2004; Hirshfeld, 1977).

Hirshfeld surface analysis was generated by *CrystalExplorer17* (Turner *et al.*, 2017; Mackenzie *et al.*, 2017) and comprised $d_{\rm norm}$ surface plots and two-dimensional (2D) fingerprint plots. The fingerprint plots provide information about the nature and types of intermolecular interactions, and their quantitative contribution to the HS. The intermolecular interactions are visualized by colour coding, *i.e.* red for short and blue for long contacts. The differences between flavanones and chalcones are shown by 2D fingerprint plots based on crystallographic data. The full fingerprint plots and those decomposed into O···H/H···O, C···C, C···H/H···C and H···H are shown in Figs. S1 and S2 (see supporting information). All chalcones display the visible participation of

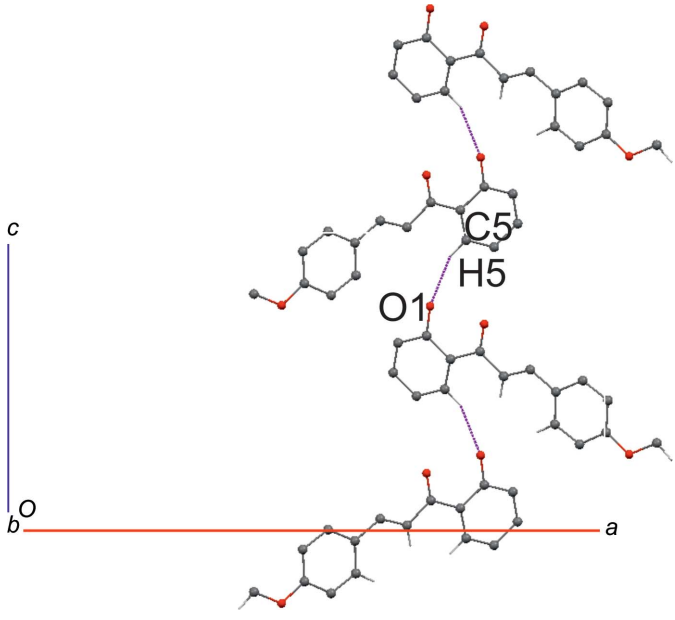


Figure 14
A fragment of the molecular structure of **CH2**, with the chain propagating along the *c* axis.

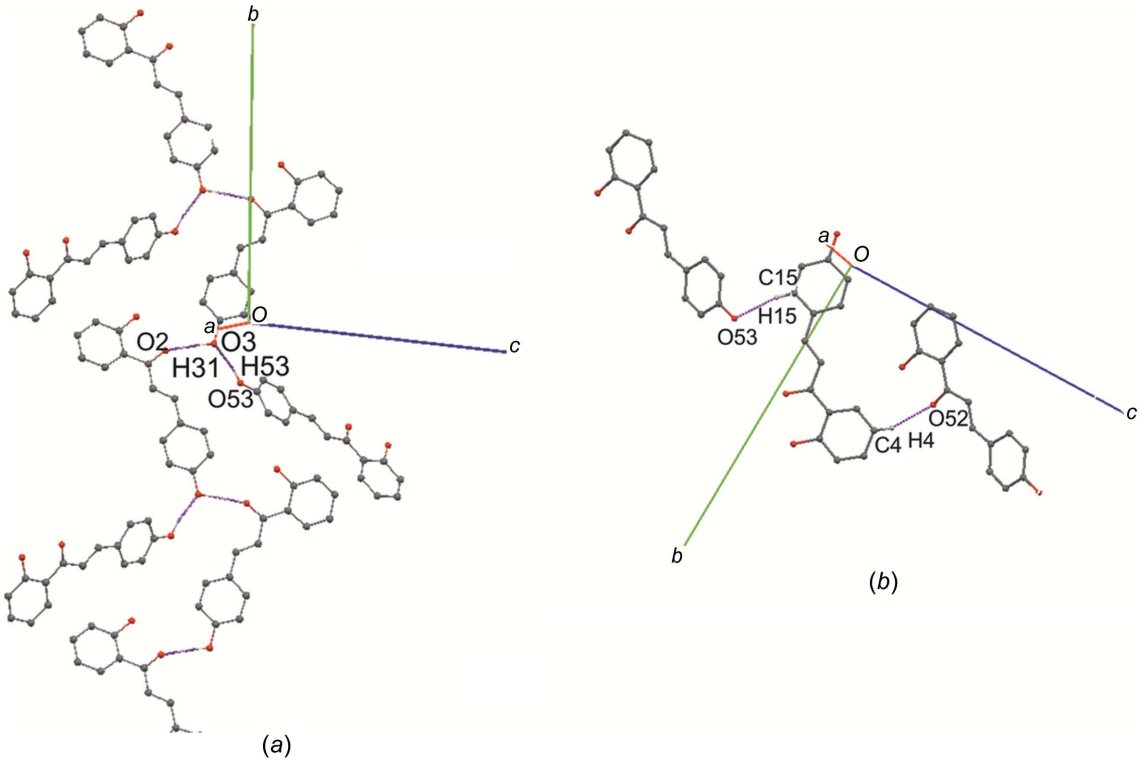


Figure 15
A fragment of the molecular structure with a net of hydrogen bonds for **CH4**. On the left is the 'fir' formed by the hydrogen bonds and, on the right, two independent molecules (pink and green) are linked into the chain.

C···C contacts due to π–π interactions which appear in the central region of the fingerprint plots (Figs. S1 and S2 in the supporting information). The reciprocal O···H interactions are present for **FL4** and **CH4** as long sharp symmetrical spikes, which can be attributed to the presence of the intermolecular interactions O3—H9···O2 in **FL4** and O3—H31···O2 and O53—H531···O3 in **CH4** (Fig. S1 and Table S1 in the supporting information). In turn, the unusual shape of the 2D fingerprint plot for **FL7** corresponds to the large number of H···H contacts associated with the presence of two methyl substituents in the *B* ring (Scheme 1).

The relative percentage contributions of the four main molecular interactions are presented in Fig. 16.

The predominant type of interaction in the studied flavanone and chalcone crystals is that of H···H close contacts. (Fig. 16*d*), which contribute between 29.3 and 48.5% of the HS, with comparable levels being observed between each pair of flavanone and chalcone isomers. A similar relationship between isomer pairs can also be observed for the contribution of O···H interactions; flavanones **FL1**–**FL4** and chalcones **CH1**–**CH4** with hydroxy or methoxy substituents at positions R^3 and R^5 demonstrate a greater percentage contribution of O···H interactions in the HS (19.4–21.8%) than **FL5**–**FL7** and **CH5**–**CH7**, which contain a halogen atom.

Figs. 16(*b*) and 16(*c*) show that, compared to other interactions, the greatest differences within each flavanone and chalcone isomer pair concern the contributions of C···C and C···H. However, in the case of **FL1**/**CH1**, **FL3**/**CH3** and **FL7**/**CH7**, the two isomers demonstrate similar percentages of C···H interactions. This may be because of all the interactions in the crystal lattice of those compounds, C—H···π and π–π are the most energetically dominant, as indicated by the decomposition of the energy frameworks (Fig. 17 and Table S4 in the supporting information). A number of π–π interactions with relatively short $Cg(I)\cdots Cg(J)$ distances for **CH2**, **CH4**, **CH5**, **CH6*A*/*B*** and **CH7**, ranging from 3.815 to 4.047 Å, are present, as reflected in the higher percentage contribution of C···C contacts in the HS (Fig. 16*b* and Table S3 in the supporting information). This is associated with the planar molecular structure of chalcones.

3.4. Energy framework analysis and lattice energy analysis

The relationship between the structural features of the compounds/isomers and their electronic descriptors/properties was enriched by the quantification of intermolecular interaction energies and the 3D topology of the interaction map. Firstly, the total interaction energy ($E_{\rm tot}^{AB}$) was calculated by the summation of the electrostatic, polarization, dispersion and exchange–repulsion energy components for each nearest-neighbour molecular pair (McKinnon *et al.*, 2007). Following this, the lattice energy ($E_{\rm lat}^{\rm CE-B3LYP}$) was estimated according to Thomas *et al.* (2018). The following trends may be observed:

(i) For seven pairs of isomers, the value of $E_{\rm lat}^{\rm CE-B3LYP}$ is greater for the flavanones than for the chalcones. In addition, the $E_{\rm lat}^{\rm CE-B3LYP}$(**FL**)/$E_{\rm lat}^{\rm CE-B3LYP}$(**CH**) ratio ranges from 0.98 to 1.14 for the five pairs **FL1**/**CH1**, **FL2**/**CH2**, **FL5**/**CH5** and **FL6**/**CH6*A*/*B*** (two polymorphs).

(ii) The opposite trend is observed in the case of pairs **FL4**/**CH4** and **FL7**/**CH7**, where the chalcones demonstrated a greater $E_{lat}^{CE-B3LYP}$ than the flavanones; this is probably due to the effect of the two independent chalcone molecules being present in an asymmetric unit, with an $E_{lat}^{CE-B3LYP}$(**FL**)/$E_{lat}^{CE-B3LYP}$(**CH**) ratio of 0.70 for **FL4**/**CH4** and 0.86 for **FL7**/**CH7**. This is also observed in the **FL3**/**CH3** pair of crystal structures, characterized by two independent molecules in the asymmetric unit; in this case, the $E_{lat}^{CE-B3LYP}$(**FL**)/$E_{lat}^{CE-B3LYP}$(**CH**) ratio is 1.63,

(iii) Two polymorphs of **CH6** have two different energies, differing by 4%; of these, the **CH6*B*** polymorph is more stable.

(iv) Most of the interactions found in the analysed structures are of the types C—H···O, C—H···π and π–π. For these, the interaction energy ranges from −19.5 to −57.4 kJ mol^{-1}; these values are comparable with the corresponding interaction energies for other structures published in Bhowal *et al.* (2019), Bal Raju *et al.* (2018) and Bhandary *et al.* (2019).

(v) The highest interaction energy is −57.4 kJ mol^{-1} (for **FL7**); this may be due to the presence of only π–π interactions in the crystal lattice, which possesses an attractive dispersive nature with small repulsion and electrostatic contribution.

(vi) C—H···Br-type hydrogen bonds and C—Br···Br- and C—Br···O-type halogen bonds are observed in two pairs (*i.e.* **CH6**/**FL6** and **CH7**/**FL7**); their pairwise interaction energies range from −4.0 to −13.3 kJ mol^{-1}. In the structures of **CH6*A*** and **FL7**, the molecules are stacked at distances of 4.002 (2) and 4.194 (4) Å; however, the spatial arrangement of these molecules differs. In the crystal structure of **CH6*A***, the molecules create a herringbone motif along the [010] direction due to the presence of a C—Br1···Br1^{i} halogen interaction [Br1···Br1^{i} = 3.715 (2) Å and C13—Br1···Br1^{i} = 167.5 (2)°; symmetry code: (i) $-x, y+\frac{1}{2}, -z+1$]; the interaction energy of this molecular pair is −9.7 kJ mol^{-1}. In the crystal structure of **FL7**, molecules form a chain along the [010] direction through the C5—H3···Br1^{ii} hydrogen bond [H3···Br1^{ii} = 2.994 (2) Å and C5—H3···Br1^{ii} = 170.2 (2)°; symmetry code: (ii) $-x+2, y+\frac{1}{2}, -z+1$], with an energy of −13.3 kJ mol^{-1}.

(vii) The energetically dominant C—H···π and π–π interactions for the pairs **FL1**/**CH1**, **FL3**/**CH3** and **FL7**/**CH7** reflect identical contributions of the C···C and C···H contacts in the HS (Figs. 16*b* and 16*c*).

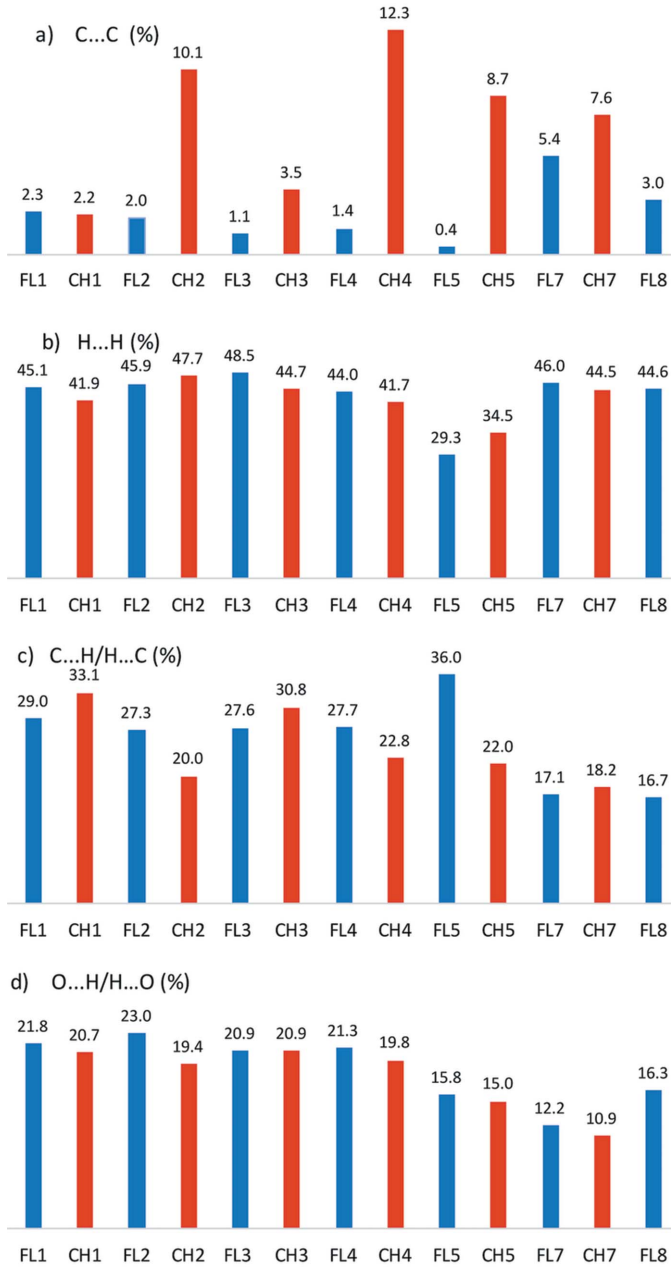


Figure 16
The relative contributions of selected intermolecular contacts to the Hirshfeld surface area in the pairs of flavanone–chalcone isomers.

3.5. Energies of the frontier molecular orbitals and global reactivity descriptors

To compare the flavanone and chalcone series, the energies of the frontier molecular orbitals were calculated, and these values were used to evaluate various global reactivity descriptors, such as chemical hardness and softness, and electrophilicity index (Siram *et al.*, 2013). The computed values of the electron structure descriptors are presented in Table S5 and a graphical representation of the electron-density redistribution is given in Table S6 (see supporting information).

Flavanones demonstrate a higher energy gap (4.531–4.861 eV) than chalcones (3.695–3.957 eV) and hence exhibit greater chemical hardness and lower electrophilicity index values. Hence, flavanones have a greater capacity to receive electrons, while the chalcones demonstrate greater resistance to their electronic configuration changing. The presence of substituents possessing either electron-withdrawing or electron-donating characters can modulate the electrophilic power of compounds. In general, electron-withdrawing groups (EWG), such as Cl or Br, will decrease the energy of the LUMO orbital, while electron-donating groups (EDG), such as OH, CH_3 and OCH_3, will increase its energy. The first four

compounds in both series (flavanones and chalcones) contain only EDGs, compounds **FL5**/**CH5** and **FL6**/**CH6** contain EWGs, whereas compounds **CH7**, **FL7** and **FL8** possess both types of substituents. All flavanones and chalcones with halogen atoms, except **CH7** (*viz*. **FL5**, **CH5**, **FL6**, **CH6**, **FL7** and **FL8**), exhibit lower values of $E_{\rm LUMO}$ than those with EDGs, and hence a higher electrophilicity index. The red colour on the electron-density redistribution plots (Table S6 in the supporting information) represents the donor parts of the molecule, *i.e.* where the electron originates, while the blue colour represents the direction in which the electrons are moving as a result of the excitation. The blue regions indicate the electrophilic sites of the molecules.

The redistribution of electron density for flavanones **FL2**, **FL3** and **FL4** show the same pattern represented by two distinct parts, the first with an electrophilic character (the whole of ring *B* with a carbonyl group in ring *A*) and the second with a nucleophilic character (the whole of ring *C*). In turn, for **FL1**, **FL5**, **FL6**, **FL7** and **FL8**, the redistribution of electrons only occurs within rings *A* and *B*. The one feature

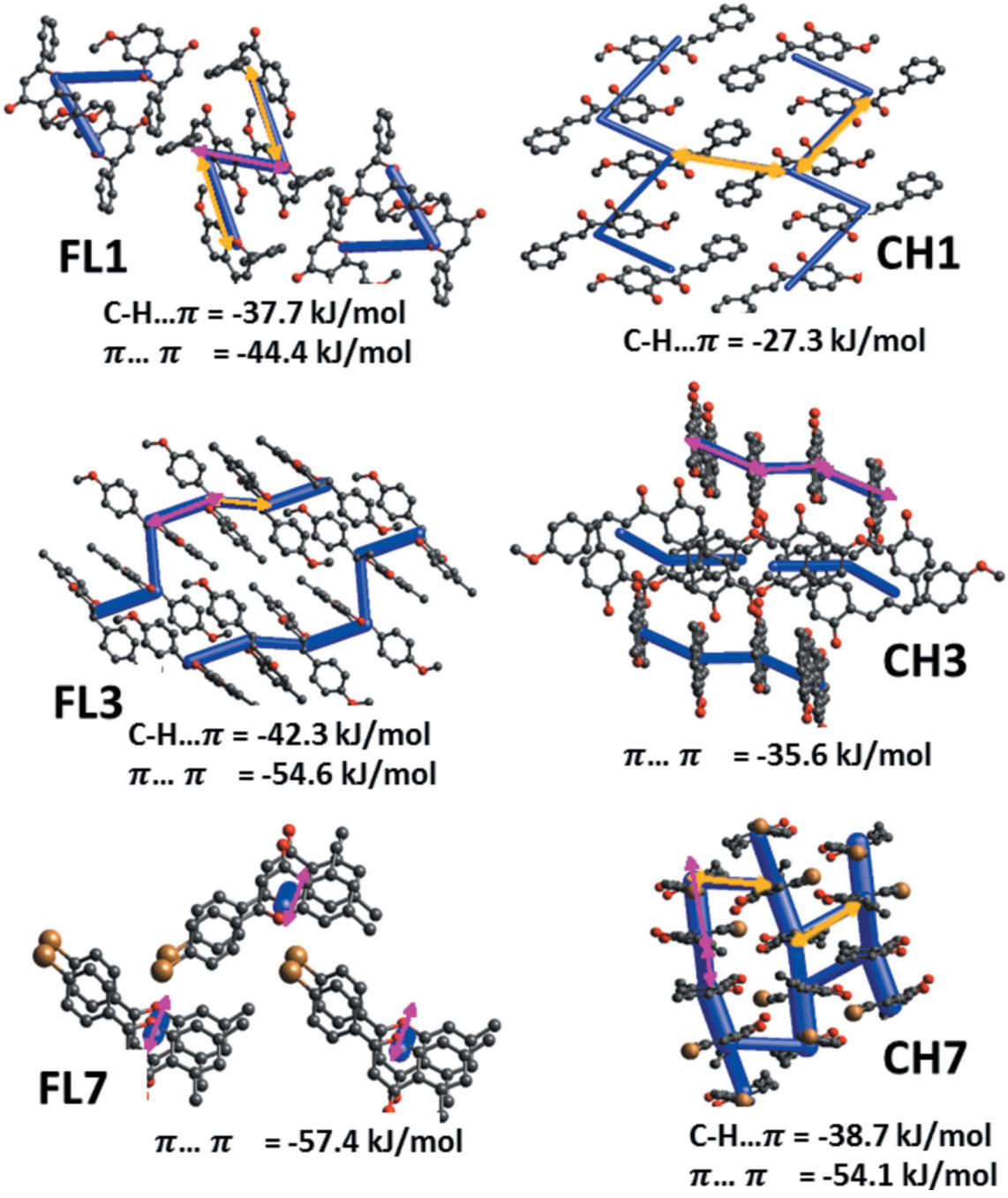


Figure 17
The energy frameworks for the pairs of crystals **FL1**/**CH1**, **FL3**/**CH3** and **FL7**/**CH7** (total energy is presented). Yellow and pink arrows indicate energetically dominant C—H$\cdots\pi$ and π–π interactions, respectively. The cutoff value is selected individually to show only one/two highest energy, if it exists.

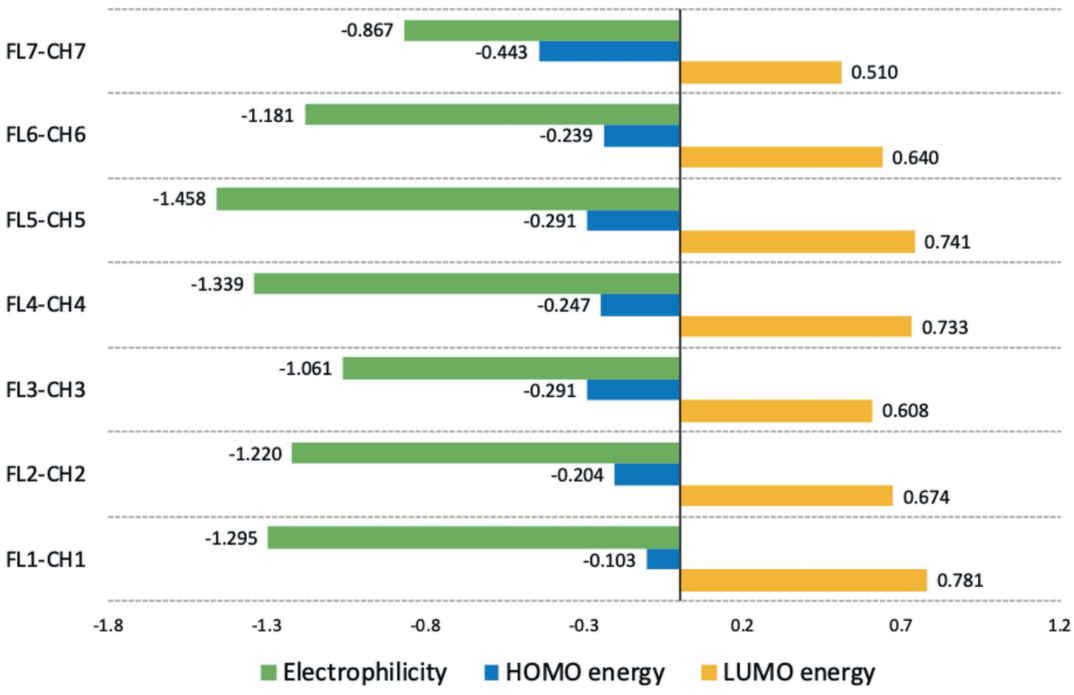


Figure 18
The difference in electrophilicity and HOMO and LUMO energies for each flavanone–chalcone pair.

common to all flavanones and chalcones is the presence of an electrophilic carbonyl group.

A comparison of the electronic properties of the analysed compounds and their intermolecular interactions, obtained using Hirshfeld surface analysis, revealed the presence of a number of relationships (Figs. S18 and S19 in the supporting information). A noticeable trend can be seen between the sum of the two most representative interactions (C···H and H···H) and the energy of the HOMO orbital or electrophilicity index. A more comprehensive analysis of the flavanone–chalcone pairs can be seen after calculating the differences between the global reactivity descriptors. Fig. 18 presents the differences in LUMO energy, HOMO energy and electrophilicity index within each pair. In the first three pairs, it can be seen that the shift of the methoxy group from the *B* ring in **FL1**/**CH1** to the *C* ring in **FL2**/**CH2**, and then the further introduction of a methyl group (in **FL3**/**CH3**) results in a gradual decrease in the absolute differences in HOMO energy, together with an increase in LUMO energy and electrophilicity. A comparable relationship can be observed for the next three pairs, *i.e.* **FL5**/**CH5**, **FL6**/**CH6** and **FL7**/**CH7**, which contain halogen atoms. Changing the Cl atom in **FL5** and **CH5** to a Br atom (**FL6**/**CH6**) causes a decrease in the LUMO energy and an increase in electrophilicity. In the **FL7**/**CH7** pair, the addition of two electron-donating groups (CH_3) increases the difference in E_{HOMO}, but the electrophilicity is lower.

4. Conclusion

The investigation of the crystal structures of a series of flavanones and chalcones indicates that weak intermolecular interactions, such as C—H···O, C—H···π and π–π, contribute to the total crystal forces. The combination of Hirshfeld surface analysis, lattice energy calculations and HOMO–LUMO investigations confirm that the energetic parameters are substantially influenced by the molecular interactions resulting from the type and position of the substituents.

It appears that, in a general sense, $E_{lat}^{CE-B3LYP}$ is greater for flavanones than for chalcones in the case of compounds with one independent molecule in the asymmetric unit. The values of the global reactivity descriptors of flavanones and chalcones result from both the nature of the substituents in the molecule (EWG or EDG) and their position. As expected, chalcones appear to be stronger electrophiles than flavanones, most likely due to the presence of an α,β-unsaturated link between the rings. However, an analysis of the electrophilicity changes within the isomers showed that as the number of substituents in the molecule increases the electrophilicity difference between the flavanone and chalcone components of the isomeric pair decreases.

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Interactions in flavanone and chalcone derivatives: Hirshfeld surface analysis, energy frameworks and global reactivity descriptors

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015) for FL1, FL2, FL3, FL5, FL8; *'CrysAlis PRO* (Rigaku OD, 2015)′ for CH2, CH4. Cell refinement: *CrysAlis PRO* (Rigaku OD, 2015) for FL1, FL2, FL3, FL5, FL8; *'CrysAlis PRO* (Rigaku OD, 2015)′ for CH2, CH4. Data reduction: *CrysAlis PRO* (Rigaku OD, 2015) for FL1, FL2, FL3, FL5, FL8; *'CrysAlis PRO* (Rigaku OD, 2015)′ for CH2, CH4. For all structures, program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015b) and *publCIF* (Westrip, 2010).

7-Methoxy-2-phenyl-3,4-dihydro-2*H*-1-benzopyran-4-one (FL1)

Crystal data

$C_{16}H_{14}O_3$
$M_r = 254.27$
Monoclinic, $P2_1/c$
$a = 8.5168$ (3) Å
$b = 6.6031$ (2) Å
$c = 23.3468$ (7) Å
$\beta = 90.737$ (3)°
$V = 1312.85$ (7) Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.286$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5133 reflections
$\theta = 3.5$–31.8°
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Prism, colourless
0.3 × 0.2 × 0.1 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: micro-focus sealed X-ray tube, SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4498 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
$T_{min} = 0.341$, $T_{max} = 1.000$
20587 measured reflections
2724 independent reflections
2550 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 26.5°$, $\theta_{min} = 3.2°$
$h = -10\rightarrow10$
$k = -6\rightarrow8$
$l = -29\rightarrow29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.112$
$S = 1.05$
2724 reflections
183 parameters
0 restraints

Primary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2 + 1.1824P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.40$ e Å^{-3}
	$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray data of five flavanone derivatives (**FL1**, **FL2**, **FL3**, **FL5** and **FL8**) were collected on a micro-focus SuperNova diffractometer with an Atlas detector, whereas data collection of two chalcone derivatives (**CH2** and **CH4**) was carried out on an Xcalibur diffractometer with a Sapphire3 detector; all using Mo *Kα* and *ω* scans at a low temperature of 100.0 (1) K. The X-ray data were corrected for absorption using *CrysAlis PRO* (Agilent, 2015). All structures were solved using SHELXT (Sheldrick, 2015a) and refined with SHELXL2014/7 (Sheldrick, 2015b). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.60169 (12)	0.27910 (16)	0.39607 (4)	0.0210 (2)	
O2	0.18209 (13)	0.31539 (17)	0.52993 (5)	0.0280 (3)	
O4	0.45378 (13)	0.80554 (18)	0.31591 (5)	0.0294 (3)	
C4	0.49738 (17)	0.6489 (2)	0.33976 (6)	0.0212 (3)	
C5	0.42163 (17)	0.5646 (2)	0.39142 (6)	0.0203 (3)	
C6	0.29195 (18)	0.6616 (2)	0.41686 (7)	0.0258 (3)	
H6	0.2560	0.7870	0.4017	0.031*	
C7	0.21647 (18)	0.5783 (2)	0.46319 (7)	0.0251 (3)	
H7	0.1303	0.6467	0.4799	0.030*	
C8	0.26814 (17)	0.3904 (2)	0.48565 (6)	0.0210 (3)	
C9	0.39774 (17)	0.2929 (2)	0.46267 (6)	0.0197 (3)	
H9	0.4341	0.1685	0.4783	0.024*	
C10	0.47402 (16)	0.3817 (2)	0.41586 (6)	0.0182 (3)	
C11	0.2223 (2)	0.1175 (3)	0.55208 (7)	0.0302 (4)	
H11A	0.2160	0.0177	0.5211	0.045*	
H11B	0.1487	0.0803	0.5823	0.045*	
H11C	0.3294	0.1203	0.5679	0.045*	
C12	0.8151 (2)	0.2302 (3)	0.33399 (8)	0.0425 (5)	
C13	0.9552 (3)	0.2792 (3)	0.36011 (7)	0.0466 (6)	
H13	0.9613	0.3919	0.3853	0.056*	
C14	1.0867 (2)	0.1648 (3)	0.34967 (8)	0.0425 (5)	
H14	1.1836	0.1990	0.3678	0.051*	
C15	1.0792 (2)	0.0001 (3)	0.31294 (7)	0.0336 (4)	
H15	1.1705	−0.0783	0.3059	0.040*	
C16	0.9390 (2)	−0.0489 (3)	0.28685 (7)	0.0340 (4)	
H16	0.9326	−0.1618	0.2617	0.041*	
C17	0.8079 (2)	0.0660 (3)	0.29730 (8)	0.0389 (5)	
H17	0.7110	0.0322	0.2791	0.047*	
C2A	0.6423 (3)	0.3149 (4)	0.33685 (12)	0.0185 (9)	0.533 (6)

H2A	0.5724	0.2316	0.3114	0.022*	0.533 (6)
C2B	0.7094 (4)	0.3986 (5)	0.36092 (14)	0.0204 (10)	0.467 (6)
H2B	0.7760	0.4845	0.3868	0.024*	0.467 (6)
C3	0.6349 (2)	0.5275 (3)	0.31836 (8)	0.0344 (4)	
H3A	0.6324	0.5306	0.2760	0.041*	0.533 (6)
H3B	0.7328	0.5957	0.3311	0.041*	0.533 (6)
H3C	0.5984	0.4420	0.2860	0.041*	0.467 (6)
H3D	0.7144	0.6224	0.3034	0.041*	0.467 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0214 (5)	0.0215 (5)	0.0203 (5)	0.0050 (4)	0.0059 (4)	0.0030 (4)
O2	0.0289 (6)	0.0270 (6)	0.0284 (6)	0.0058 (5)	0.0132 (5)	0.0071 (5)
O4	0.0283 (6)	0.0288 (6)	0.0311 (6)	0.0065 (5)	0.0048 (5)	0.0113 (5)
C4	0.0203 (7)	0.0223 (7)	0.0208 (7)	0.0010 (6)	−0.0005 (5)	0.0018 (6)
C5	0.0207 (7)	0.0218 (7)	0.0185 (7)	0.0024 (6)	0.0008 (5)	0.0007 (6)
C6	0.0278 (8)	0.0238 (8)	0.0258 (8)	0.0078 (6)	0.0037 (6)	0.0047 (6)
C7	0.0238 (7)	0.0264 (8)	0.0251 (7)	0.0072 (6)	0.0059 (6)	0.0006 (6)
C8	0.0212 (7)	0.0233 (7)	0.0186 (7)	−0.0009 (6)	0.0030 (5)	0.0007 (6)
C9	0.0217 (7)	0.0184 (7)	0.0192 (7)	0.0019 (6)	0.0007 (5)	0.0008 (6)
C10	0.0175 (6)	0.0200 (7)	0.0172 (6)	0.0010 (5)	0.0000 (5)	−0.0032 (5)
C11	0.0379 (9)	0.0242 (8)	0.0290 (8)	0.0010 (7)	0.0125 (7)	0.0060 (7)
C12	0.0480 (11)	0.0427 (11)	0.0374 (10)	0.0269 (9)	0.0279 (9)	0.0241 (9)
C13	0.1000 (18)	0.0214 (8)	0.0187 (8)	−0.0007 (10)	0.0113 (9)	−0.0015 (7)
C14	0.0436 (10)	0.0533 (12)	0.0301 (9)	−0.0232 (10)	−0.0160 (8)	0.0189 (9)
C15	0.0298 (8)	0.0418 (10)	0.0295 (8)	0.0172 (7)	0.0140 (7)	0.0181 (8)
C16	0.0612 (12)	0.0215 (8)	0.0195 (7)	−0.0040 (8)	0.0036 (7)	−0.0014 (6)
C17	0.0246 (8)	0.0529 (12)	0.0391 (10)	−0.0121 (8)	−0.0064 (7)	0.0252 (9)
C2A	0.0202 (15)	0.0208 (15)	0.0147 (14)	0.0021 (12)	0.0037 (11)	0.0004 (11)
C2B	0.0205 (17)	0.0217 (17)	0.0190 (16)	−0.0009 (14)	0.0023 (13)	−0.0021 (13)
C3	0.0339 (9)	0.0373 (10)	0.0324 (9)	0.0134 (8)	0.0162 (7)	0.0155 (8)

Geometric parameters (Å, º)

O1—C10	1.3666 (17)	C12—C17	1.383 (3)
O1—C2A	1.449 (3)	C12—C2B	1.567 (4)
O1—C2B	1.469 (3)	C12—C2A	1.577 (3)
O2—C8	1.3676 (17)	C13—C14	1.376 (3)
O2—C11	1.4448 (19)	C13—H13	0.9500
O4—C4	1.2299 (19)	C14—C15	1.386 (3)
C4—C5	1.483 (2)	C14—H14	0.9500
C4—C3	1.509 (2)	C15—C16	1.372 (3)
C5—C10	1.406 (2)	C15—H15	0.9500
C5—C6	1.414 (2)	C16—C17	1.375 (3)
C6—C7	1.380 (2)	C16—H16	0.9500
C6—H6	0.9500	C17—H17	0.9500
C7—C8	1.415 (2)	C2A—C3	1.470 (3)

C7—H7	0.9500	C2A—H2A	1.0000
C8—C9	1.391 (2)	C2B—C3	1.449 (4)
C9—C10	1.406 (2)	C2B—H2B	1.0000
C9—H9	0.9500	C3—H3A	0.9900
C11—H11A	0.9800	C3—H3B	0.9900
C11—H11B	0.9800	C3—H3C	0.9900
C11—H11C	0.9800	C3—H3D	0.9900
C12—C13	1.372 (3)		

C10—O1—C2A	116.25 (14)	C14—C13—H13	120.1
C10—O1—C2B	115.34 (16)	C13—C14—C15	120.63 (17)
C8—O2—C11	118.11 (12)	C13—C14—H14	119.7
O4—C4—C5	123.48 (14)	C15—C14—H14	119.7
O4—C4—C3	121.85 (14)	C16—C15—C14	119.53 (16)
C5—C4—C3	114.67 (13)	C16—C15—H15	120.2
C10—C5—C6	117.64 (13)	C14—C15—H15	120.2
C10—C5—C4	120.87 (13)	C15—C16—C17	119.67 (16)
C6—C5—C4	121.46 (13)	C15—C16—H16	120.2
C7—C6—C5	121.54 (14)	C17—C16—H16	120.2
C7—C6—H6	119.2	C16—C17—C12	120.88 (17)
C5—C6—H6	119.2	C16—C17—H17	119.6
C6—C7—C8	119.62 (14)	C12—C17—H17	119.6
C6—C7—H7	120.2	O1—C2A—C3	115.2 (2)
C8—C7—H7	120.2	O1—C2A—C12	102.52 (18)
O2—C8—C9	124.03 (14)	C3—C2A—C12	111.3 (2)
O2—C8—C7	115.50 (13)	O1—C2A—H2A	109.2
C9—C8—C7	120.47 (13)	C3—C2A—H2A	109.2
C8—C9—C10	118.92 (13)	C12—C2A—H2A	109.2
C8—C9—H9	120.5	C3—C2B—O1	115.3 (2)
C10—C9—H9	120.5	C3—C2B—C12	113.0 (2)
O1—C10—C5	122.58 (13)	O1—C2B—C12	102.1 (2)
O1—C10—C9	115.69 (13)	C3—C2B—H2B	108.7
C5—C10—C9	121.74 (13)	O1—C2B—H2B	108.7
O2—C11—H11A	109.5	C12—C2B—H2B	108.7
O2—C11—H11B	109.5	C2B—C3—C4	114.84 (17)
H11A—C11—H11B	109.5	C2A—C3—C4	116.13 (16)
O2—C11—H11C	109.5	C2A—C3—H3A	108.3
H11A—C11—H11C	109.5	C4—C3—H3A	108.3
H11B—C11—H11C	109.5	C2A—C3—H3B	108.3
C13—C12—C17	119.47 (16)	C4—C3—H3B	108.3
C13—C12—C2B	98.9 (2)	H3A—C3—H3B	107.4
C17—C12—C2B	141.6 (2)	C2B—C3—H3C	108.6
C13—C12—C2A	134.8 (2)	C4—C3—H3C	108.6
C17—C12—C2A	105.7 (2)	C2B—C3—H3D	108.6
C12—C13—C14	119.82 (17)	C4—C3—H3D	108.6
C12—C13—H13	120.1	H3C—C3—H3D	107.5

O4—C4—C5—C10	178.20 (14)	C13—C14—C15—C16	0.0 (3)

C3—C4—C5—C10	−2.2 (2)	C14—C15—C16—C17	0.2 (2)
O4—C4—C5—C6	0.0 (2)	C15—C16—C17—C12	−0.3 (3)
C3—C4—C5—C6	179.58 (15)	C13—C12—C17—C16	0.2 (3)
C10—C5—C6—C7	−1.5 (2)	C2B—C12—C17—C16	−177.9 (2)
C4—C5—C6—C7	176.75 (15)	C2A—C12—C17—C16	−177.50 (17)
C5—C6—C7—C8	−0.7 (2)	C10—O1—C2A—C3	42.9 (3)
C11—O2—C8—C9	−3.8 (2)	C10—O1—C2A—C12	163.97 (15)
C11—O2—C8—C7	175.80 (14)	C13—C12—C2A—O1	−62.3 (3)
C6—C7—C8—O2	−177.26 (14)	C17—C12—C2A—O1	114.88 (19)
C6—C7—C8—C9	2.3 (2)	C13—C12—C2A—C3	61.4 (3)
O2—C8—C9—C10	177.95 (13)	C17—C12—C2A—C3	−121.4 (2)
C7—C8—C9—C10	−1.6 (2)	C10—O1—C2B—C3	−44.2 (3)
C2A—O1—C10—C5	−24.6 (2)	C10—O1—C2B—C12	−167.06 (16)
C2B—O1—C10—C5	18.7 (2)	C13—C12—C2B—C3	121.6 (2)
C2A—O1—C10—C9	155.59 (18)	C17—C12—C2B—C3	−60.0 (4)
C2B—O1—C10—C9	−161.12 (19)	C13—C12—C2B—O1	−113.9 (2)
C6—C5—C10—O1	−177.56 (13)	C17—C12—C2B—O1	64.5 (3)
C4—C5—C10—O1	4.2 (2)	O1—C2B—C3—C4	45.8 (3)
C6—C5—C10—C9	2.3 (2)	C12—C2B—C3—C4	162.6 (2)
C4—C5—C10—C9	−176.02 (13)	O1—C2A—C3—C4	−41.0 (3)
C8—C9—C10—O1	179.09 (12)	C12—C2A—C3—C4	−157.19 (18)
C8—C9—C10—C5	−0.7 (2)	O4—C4—C3—C2B	157.1 (2)
C17—C12—C13—C14	−0.1 (3)	C5—C4—C3—C2B	−22.5 (3)
C2B—C12—C13—C14	178.76 (19)	O4—C4—C3—C2A	−159.74 (19)
C2A—C12—C13—C14	176.8 (2)	C5—C4—C3—C2A	20.7 (3)
C12—C13—C14—C15	0.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O4^{i}	0.95	2.64	3.439 (3)	158

Symmetry code: (i) *x*+1, *y*−1, *z*.

2-(4-Methoxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-4-one (FL2)

Crystal data

$C_{16}H_{14}O_3$
M_r = 254.27
Orthorhombic, *Pbcn*
a = 12.7692 (2) Å
b = 8.5258 (1) Å
c = 23.1820 (3) Å
V = 2523.77 (6) Å^3
Z = 8
F(000) = 1072

D_x = 1.338 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 10611 reflections
θ = 3.4–35.7°
μ = 0.09 mm^{-1}
T = 100 K
Prism, colourless
0.4 × 0.2 × 0.1 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: micro-focus sealed X-ray tube, SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4498 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.671, T_{max} = 1.000
19929 measured reflections
2615 independent reflections
2267 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.5°, θ_{min} = 3.0°
h = −16→16
k = −9→10
l = −28→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.144
S = 1.03
2615 reflections
183 parameters
3 restraints
Primary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 2.4485P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray data of five flavanone derivatives (**FL1**, **FL2**, **FL3**, **FL5** and **FL8**) were collected on a micro-focus SuperNova diffractometer with an Atlas detector, whereas data collection of two chalcone derivatives (**CH2** and **CH4**) was carried out on an Xcalibur diffractometer with a Sapphire3 detector; all using Mo $K\alpha$ and ω scans at a low temperature of 100.0 (1) K. The X-ray data were corrected for absorption using *CrysAlis PRO* (Agilent, 2015). All structures were solved using SHELXT (Sheldrick, 2015a) and refined with SHELXL2014/7 (Sheldrick, 2015b). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.37524 (9)	0.14801 (14)	0.58084 (5)	0.0276 (3)	
O2	0.85340 (10)	0.11366 (18)	0.64971 (6)	0.0374 (4)	
O4	0.18991 (11)	−0.08707 (19)	0.69662 (6)	0.0439 (4)	
C4	0.24514 (15)	−0.0228 (2)	0.66092 (8)	0.0326 (4)	
C5	0.20276 (14)	0.0562 (2)	0.60943 (8)	0.0274 (4)	
C6	0.09534 (15)	0.0504 (2)	0.59704 (9)	0.0343 (4)	
H6	0.0496	−0.0060	0.6218	0.041*	
C7	0.05564 (16)	0.1258 (2)	0.54939 (10)	0.0396 (5)	
H7	−0.0172	0.1214	0.5412	0.048*	
C8	0.12270 (16)	0.2083 (3)	0.51319 (9)	0.0413 (5)	
H8	0.0951	0.2600	0.4802	0.050*	
C9	0.22914 (15)	0.2163 (2)	0.52445 (8)	0.0345 (4)	
H9	0.2741	0.2741	0.4997	0.041*	
C10	0.26957 (13)	0.13885 (19)	0.57245 (7)	0.0259 (4)	

C12	0.53084 (16)	0.0909 (4)	0.63301 (11)	0.0615 (8)	
C13	0.59748 (17)	0.0045 (3)	0.59844 (10)	0.0486 (6)	
H13	0.5689	−0.0635	0.5700	0.058*	
C14	0.70479 (15)	0.0150 (2)	0.60446 (8)	0.0336 (4)	
H14	0.7496	−0.0441	0.5800	0.040*	
C15	0.74675 (14)	0.1122 (2)	0.64637 (7)	0.0280 (4)	
C16	0.68152 (17)	0.2008 (2)	0.68107 (9)	0.0408 (5)	
H16	0.7101	0.2684	0.7096	0.049*	
C17	0.57444 (19)	0.1900 (3)	0.67388 (11)	0.0566 (7)	
H17	0.5297	0.2518	0.6974	0.068*	
C18	0.89804 (19)	0.1915 (3)	0.69807 (9)	0.0567 (7)	
H18A	0.8797	0.3031	0.6968	0.085*	
H18B	0.9744	0.1801	0.6970	0.085*	
H18C	0.8708	0.1450	0.7337	0.085*	
C2A	0.4103 (2)	0.1137 (3)	0.63910 (13)	0.0241 (10)	0.526 (7)
H2A	0.3978	0.2089	0.6633	0.029*	0.526 (7)
C2B	0.4192 (2)	0.0302 (4)	0.61717 (12)	0.0279 (12)	0.474 (7)
H2B	0.4287	−0.0657	0.5929	0.033*	0.474 (7)
C3	0.36129 (17)	−0.0153 (4)	0.66630 (10)	0.0617 (8)	
H3A	0.3793	−0.0128	0.7078	0.074*	0.526 (7)
H3B	0.3911	−0.1129	0.6500	0.074*	0.526 (7)
H3C	0.3782	0.0587	0.6979	0.074*	0.474 (7)
H3D	0.3864	−0.1201	0.6784	0.074*	0.474 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0277 (6)	0.0314 (7)	0.0236 (6)	−0.0022 (5)	−0.0015 (5)	0.0043 (5)
O2	0.0269 (7)	0.0527 (9)	0.0326 (7)	−0.0106 (6)	−0.0012 (5)	−0.0044 (6)
O4	0.0405 (8)	0.0533 (9)	0.0380 (8)	−0.0070 (7)	0.0092 (6)	0.0104 (7)
C4	0.0343 (9)	0.0334 (9)	0.0302 (9)	−0.0041 (8)	0.0032 (8)	0.0018 (7)
C5	0.0293 (9)	0.0217 (8)	0.0313 (9)	0.0019 (7)	0.0015 (7)	−0.0040 (7)
C6	0.0298 (9)	0.0261 (9)	0.0471 (11)	0.0002 (7)	0.0023 (8)	−0.0019 (8)
C7	0.0316 (10)	0.0338 (10)	0.0535 (12)	0.0011 (8)	−0.0088 (9)	−0.0055 (9)
C8	0.0424 (11)	0.0425 (11)	0.0391 (11)	0.0023 (9)	−0.0139 (9)	0.0026 (9)
C9	0.0389 (11)	0.0371 (10)	0.0275 (9)	−0.0018 (8)	−0.0049 (8)	0.0011 (7)
C10	0.0281 (9)	0.0235 (8)	0.0261 (8)	0.0008 (7)	−0.0020 (7)	−0.0047 (6)
C12	0.0247 (10)	0.102 (2)	0.0580 (14)	0.0043 (12)	0.0037 (10)	0.0554 (15)
C13	0.0384 (11)	0.0640 (14)	0.0433 (11)	−0.0222 (11)	−0.0151 (9)	0.0192 (11)
C14	0.0330 (9)	0.0365 (10)	0.0315 (9)	−0.0034 (8)	−0.0016 (7)	−0.0010 (8)
C15	0.0264 (8)	0.0302 (9)	0.0274 (8)	−0.0046 (7)	0.0028 (7)	0.0024 (7)
C16	0.0534 (12)	0.0334 (10)	0.0356 (10)	0.0005 (9)	0.0156 (9)	0.0020 (8)
C17	0.0473 (13)	0.0677 (16)	0.0549 (14)	0.0277 (12)	0.0276 (11)	0.0330 (13)
C18	0.0546 (14)	0.0864 (19)	0.0291 (10)	−0.0389 (13)	−0.0094 (9)	0.0048 (11)
C2A	0.0302 (18)	0.0223 (18)	0.0198 (16)	0.0054 (13)	0.0008 (12)	−0.0027 (13)
C2B	0.0276 (19)	0.027 (2)	0.029 (2)	0.0065 (15)	0.0015 (15)	0.0038 (17)
C3	0.0374 (12)	0.097 (2)	0.0504 (13)	−0.0251 (13)	−0.0147 (10)	0.0452 (14)

Geometric parameters (Å, º)

O1—C10	1.365 (2)	C12—C2B	1.561 (3)
O1—C2B	1.426 (3)	C13—C14	1.380 (3)
O1—C2A	1.453 (3)	C13—H13	0.9500
O2—C15	1.364 (2)	C14—C15	1.385 (3)
O2—C18	1.422 (2)	C14—H14	0.9500
O4—C4	1.218 (2)	C15—C16	1.382 (3)
C4—C5	1.474 (2)	C16—C17	1.381 (3)
C4—C3	1.490 (3)	C16—H16	0.9500
C5—C10	1.400 (2)	C17—H17	0.9500
C5—C6	1.402 (3)	C18—H18A	0.9800
C6—C7	1.375 (3)	C18—H18B	0.9800
C6—H6	0.9500	C18—H18C	0.9800
C7—C8	1.390 (3)	C2A—C3	1.414 (3)
C7—H7	0.9500	C2A—H2A	1.0000
C8—C9	1.386 (3)	C2B—C3	1.412 (3)
C8—H8	0.9500	C2B—H2B	1.0000
C9—C10	1.393 (2)	C3—H3A	0.9900
C9—H9	0.9500	C3—H3B	0.9900
C12—C13	1.382 (4)	C3—H3C	0.9900
C12—C17	1.386 (4)	C3—H3D	0.9900
C12—C2A	1.558 (3)		

C10—O1—C2B	115.64 (15)	C16—C15—C14	120.13 (19)
C10—O1—C2A	115.19 (15)	C17—C16—C15	119.4 (2)
C15—O2—C18	116.69 (16)	C17—C16—H16	120.3
O4—C4—C5	122.93 (18)	C15—C16—H16	120.3
O4—C4—C3	122.62 (18)	C16—C17—C12	121.4 (2)
C5—C4—C3	114.43 (16)	C16—C17—H17	119.3
C10—C5—C6	119.24 (16)	C12—C17—H17	119.3
C10—C5—C4	120.16 (16)	O2—C18—H18A	109.5
C6—C5—C4	120.59 (17)	O2—C18—H18B	109.5
C7—C6—C5	120.59 (18)	H18A—C18—H18B	109.5
C7—C6—H6	119.7	O2—C18—H18C	109.5
C5—C6—H6	119.7	H18A—C18—H18C	109.5
C6—C7—C8	119.63 (18)	H18B—C18—H18C	109.5
C6—C7—H7	120.2	C3—C2A—O1	115.8 (2)
C8—C7—H7	120.2	C3—C2A—C12	112.37 (19)
C9—C8—C7	121.03 (18)	O1—C2A—C12	104.21 (18)
C9—C8—H8	119.5	C3—C2A—H2A	108.1
C7—C8—H8	119.5	O1—C2A—H2A	108.1
C8—C9—C10	119.37 (18)	C12—C2A—H2A	108.1
C8—C9—H9	120.3	C3—C2B—O1	117.6 (2)
C10—C9—H9	120.3	C3—C2B—C12	112.29 (19)
O1—C10—C9	116.92 (15)	O1—C2B—C12	105.4 (2)
O1—C10—C5	122.95 (15)	C3—C2B—H2B	107.0
C9—C10—C5	120.13 (16)	O1—C2B—H2B	107.0

C13—C12—C17	118.3 (2)	C12—C2B—H2B	107.0
C13—C12—C2A	136.7 (3)	C2B—C3—C4	117.73 (19)
C17—C12—C2A	105.0 (2)	C2A—C3—C4	115.9 (2)
C13—C12—C2B	104.4 (2)	C2A—C3—H3A	108.3
C17—C12—C2B	136.9 (2)	C4—C3—H3A	108.3
C12—C13—C14	121.2 (2)	C2A—C3—H3B	108.3
C12—C13—H13	119.4	C4—C3—H3B	108.3
C14—C13—H13	119.4	H3A—C3—H3B	107.4
C13—C14—C15	119.6 (2)	C2B—C3—H3C	107.9
C13—C14—H14	120.2	C4—C3—H3C	107.9
C15—C14—H14	120.2	C2B—C3—H3D	107.9
O2—C15—C16	124.30 (17)	C4—C3—H3D	107.9
O2—C15—C14	115.56 (16)	H3C—C3—H3D	107.2

O4—C4—C5—C10	174.82 (18)	O2—C15—C16—C17	180.00 (18)
C3—C4—C5—C10	−4.2 (3)	C14—C15—C16—C17	0.7 (3)
O4—C4—C5—C6	−4.8 (3)	C15—C16—C17—C12	0.7 (3)
C3—C4—C5—C6	176.2 (2)	C13—C12—C17—C16	−1.3 (3)
C10—C5—C6—C7	−0.4 (3)	C2A—C12—C17—C16	179.9 (2)
C4—C5—C6—C7	179.21 (17)	C2B—C12—C17—C16	170.3 (3)
C5—C6—C7—C8	0.0 (3)	C10—O1—C2A—C3	42.2 (3)
C6—C7—C8—C9	−0.2 (3)	C10—O1—C2A—C12	166.16 (18)
C7—C8—C9—C10	0.7 (3)	C13—C12—C2A—C3	75.4 (4)
C2B—O1—C10—C9	−160.1 (2)	C17—C12—C2A—C3	−106.2 (2)
C2A—O1—C10—C9	160.29 (18)	C13—C12—C2A—O1	−50.7 (3)
C2B—O1—C10—C5	19.8 (3)	C17—C12—C2A—O1	127.7 (2)
C2A—O1—C10—C5	−19.9 (2)	C10—O1—C2B—C3	−39.2 (3)
C8—C9—C10—O1	178.71 (17)	C10—O1—C2B—C12	−165.24 (17)
C8—C9—C10—C5	−1.2 (3)	C13—C12—C2B—C3	127.8 (3)
C6—C5—C10—O1	−178.86 (15)	C17—C12—C2B—C3	−44.6 (4)
C4—C5—C10—O1	1.5 (2)	C13—C12—C2B—O1	−102.9 (2)
C6—C5—C10—C9	1.0 (3)	C17—C12—C2B—O1	84.7 (3)
C4—C5—C10—C9	−178.64 (16)	O1—C2B—C3—C4	36.9 (4)
C17—C12—C13—C14	0.5 (3)	C12—C2B—C3—C4	159.5 (3)
C2A—C12—C13—C14	178.8 (2)	O1—C2A—C3—C4	−45.7 (3)
C2B—C12—C13—C14	−173.6 (2)	C12—C2A—C3—C4	−165.2 (2)
C12—C13—C14—C15	0.9 (3)	O4—C4—C3—C2B	166.2 (2)
C18—O2—C15—C16	10.7 (3)	C5—C4—C3—C2B	−14.8 (3)
C18—O2—C15—C14	−169.96 (18)	O4—C4—C3—C2A	−152.8 (2)
C13—C14—C15—O2	179.15 (17)	C5—C4—C3—C2A	26.1 (3)
C13—C14—C15—C16	−1.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O4^{i}	0.95	2.51	3.365 (3)	149

C2*A*—H2*A*···O4^{ii}	1.00	2.21	3.150 (3)	156

Symmetry codes: (i) *x*+1/2, *y*+1/2, −*z*+3/2; (ii) −*x*+1/2, *y*+1/2, *z*.

2-(4-Methoxyphenyl)-6-methyl-3,4-dihydro-2*H*-1-benzopyran-4-one (FL3)

Crystal data

$C_{17}H_{16}O_3$
M_r = 268.30
Monoclinic, $P2_1/n$
a = 16.7561 (3) Å
b = 8.0448 (1) Å
c = 21.3319 (4) Å
β = 110.138 (2)°
V = 2699.74 (8) Å^3
Z = 8
F(000) = 1136
D_x = 1.320 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 12573 reflections
θ = 3.6–39.6°
μ = 0.09 mm^{-1}
T = 100 K
Prism, colourless
0.3 × 0.2 × 0.1 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: micro-focus sealed X-ray tube, SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4498 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.752, T_{max} = 1.000
21035 measured reflections
5586 independent reflections
4898 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 26.5°, θ_{min} = 2.9°
h = −21→17
k = −10→9
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 1.03
5586 reflections
391 parameters
5 restraints
Primary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 1.780P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray data of five flavanone derivatives (**FL1**, **FL2**, **FL3**, **FL5** and **FL8**) were collected on a micro-focus SuperNova diffractometer with an Atlas detector, whereas data collection of two chalcone derivatives (**CH2** and **CH4**) was carried out on an Xcalibur diffractometer with a Sapphire3 detector; all using Mo *Kα* and *ω* scans at a low temperature of 100.0 (1) K. The X-ray data were corrected for absorption using *CrysAlis PRO* (Agilent, 2015). All structures were solved using SHELXT (Sheldrick, 2015a) and refined with SHELXL2014/7 (Sheldrick, 2015b). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.93501 (6)	0.43575 (12)	0.37957 (5)	0.0233 (2)	
O2	0.54766 (7)	0.58037 (14)	0.23161 (6)	0.0329 (3)	
O4	1.08460 (8)	0.85266 (14)	0.42977 (7)	0.0426 (3)	
C2A	0.90139 (17)	0.5977 (3)	0.3841 (2)	0.0166 (8)	0.549 (7)
H2A	0.9024	0.6171	0.4307	0.020*	0.549 (7)
C3A	0.94944 (15)	0.7382 (3)	0.36373 (18)	0.0210 (8)	0.549 (7)
H3A	0.9235	0.8474	0.3662	0.025*	0.549 (7)
H3B	0.9492	0.7212	0.3177	0.025*	0.549 (7)
C2B	0.9028 (2)	0.5952 (4)	0.3525 (3)	0.0273 (11)	0.451 (7)
H2B	0.9154	0.6125	0.3104	0.033*	0.451 (7)
C3B	0.94369 (14)	0.7304 (4)	0.4000 (3)	0.0300 (13)	0.451 (7)
H3C	0.9319	0.7151	0.4420	0.036*	0.451 (7)
H3D	0.9200	0.8391	0.3806	0.036*	0.451 (7)
C4	1.04103 (10)	0.7280 (2)	0.41481 (9)	0.0363 (4)	
C5	1.07587 (9)	0.55827 (17)	0.42790 (7)	0.0203 (3)	
C6	1.16360 (9)	0.53184 (18)	0.45720 (7)	0.0207 (3)	
H6	1.2004	0.6250	0.4707	0.025*	
C7	1.19798 (9)	0.37352 (18)	0.46702 (7)	0.0201 (3)	
C8	1.14183 (9)	0.23843 (18)	0.44596 (7)	0.0207 (3)	
H8	1.1643	0.1288	0.4514	0.025*	
C9	1.05490 (9)	0.26039 (17)	0.41753 (7)	0.0211 (3)	
H9	1.0183	0.1669	0.4042	0.025*	
C10	1.02144 (9)	0.42092 (17)	0.40862 (7)	0.0192 (3)	
C11	1.29227 (9)	0.3442 (2)	0.49896 (7)	0.0250 (3)	
H11A	1.3220	0.4512	0.5075	0.037*	
H11B	1.3124	0.2777	0.4689	0.037*	
H11C	1.3036	0.2845	0.5412	0.037*	
C12	0.80738 (9)	0.59108 (18)	0.33540 (9)	0.0308 (4)	
C13	0.75563 (10)	0.49805 (18)	0.36045 (7)	0.0247 (3)	
H13	0.7804	0.4378	0.4008	0.030*	
C14	0.66838 (9)	0.49090 (17)	0.32784 (7)	0.0213 (3)	
H14	0.6337	0.4268	0.3458	0.026*	
C15	0.63221 (9)	0.57846 (17)	0.26866 (7)	0.0196 (3)	
C16	0.68325 (9)	0.67314 (18)	0.24306 (7)	0.0225 (3)	
H16	0.6585	0.7337	0.2028	0.027*	
C17	0.76978 (10)	0.67892 (19)	0.27625 (9)	0.0289 (3)	
H17	0.8044	0.7439	0.2585	0.035*	
C18	0.49235 (11)	0.4864 (3)	0.25648 (13)	0.0547 (6)	
H18A	0.5107	0.3700	0.2620	0.082*	
H18B	0.4340	0.4932	0.2248	0.082*	
H18C	0.4945	0.5317	0.2997	0.082*	
O51	0.36187 (6)	0.17192 (12)	0.21123 (5)	0.0216 (2)	
O52	0.71873 (7)	0.11084 (14)	0.43352 (5)	0.0276 (2)	
O54	0.21703 (7)	−0.24907 (13)	0.16086 (5)	0.0263 (2)	
C52A	0.37855 (10)	0.03419 (19)	0.25971 (8)	0.0202 (4)	0.932 (3)

H52A	0.3425	0.0514	0.2880	0.024*	0.932 (3)
C53A	0.35236 (10)	−0.12833 (19)	0.22231 (8)	0.0213 (4)	0.932 (3)
H53A	0.3624	−0.2212	0.2545	0.026*	0.932 (3)
H53B	0.3871	−0.1479	0.1937	0.026*	0.932 (3)
C52B	0.4030 (11)	0.0116 (9)	0.2363 (6)	0.0202 (4)	0.068 (3)
H52B	0.4274	−0.0415	0.2045	0.024*	0.068 (3)
C53B	0.3300 (12)	−0.092 (3)	0.2452 (7)	0.0213 (4)	0.068 (3)
H53C	0.3528	−0.2003	0.2657	0.026*	0.068 (3)
H53D	0.3069	−0.0331	0.2759	0.026*	0.068 (3)
C54	0.25884 (9)	−0.12241 (18)	0.17932 (7)	0.0217 (3)	
C55	0.22381 (9)	0.04487 (18)	0.15735 (7)	0.0202 (3)	
C56	0.13815 (9)	0.06681 (18)	0.11817 (7)	0.0217 (3)	
H56	0.1010	−0.0262	0.1095	0.026*	
C57	0.10606 (9)	0.22006 (19)	0.09179 (7)	0.0227 (3)	
C58	0.16332 (9)	0.35324 (19)	0.10363 (7)	0.0243 (3)	
H58	0.1433	0.4582	0.0842	0.029*	
C59	0.24797 (9)	0.33659 (18)	0.14273 (7)	0.0239 (3)	
H59	0.2852	0.4293	0.1502	0.029*	
C60	0.27838 (9)	0.18274 (18)	0.17123 (7)	0.0200 (3)	
C61	0.01240 (9)	0.2432 (2)	0.05307 (8)	0.0282 (3)	
H61A	−0.0116	0.1387	0.0310	0.042*	
H61B	0.0050	0.3303	0.0194	0.042*	
H61C	−0.0170	0.2758	0.0837	0.042*	
C62	0.47052 (9)	0.04642 (18)	0.30397 (8)	0.0243 (3)	
C63	0.53657 (10)	−0.0287 (2)	0.28915 (8)	0.0285 (3)	
H63	0.5241	−0.0934	0.2497	0.034*	
C64	0.62090 (9)	−0.01086 (19)	0.33126 (8)	0.0264 (3)	
H64	0.6655	−0.0629	0.3206	0.032*	
C65	0.63882 (9)	0.08347 (18)	0.38873 (7)	0.0217 (3)	
C66	0.57303 (10)	0.15820 (19)	0.40451 (8)	0.0255 (3)	
H66	0.5853	0.2218	0.4442	0.031*	
C67	0.49030 (10)	0.13952 (18)	0.36242 (8)	0.0261 (3)	
H67	0.4458	0.1911	0.3734	0.031*	
C68	0.78807 (9)	0.0417 (2)	0.41763 (8)	0.0309 (4)	
H68A	0.7827	−0.0797	0.4152	0.046*	
H68B	0.8418	0.0721	0.4524	0.046*	
H68C	0.7872	0.0851	0.3745	0.046*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0177 (5)	0.0144 (5)	0.0316 (6)	0.0001 (4)	0.0004 (4)	−0.0026 (4)
O2	0.0201 (5)	0.0243 (6)	0.0439 (7)	−0.0035 (4)	−0.0021 (5)	0.0079 (5)
O4	0.0319 (6)	0.0160 (6)	0.0611 (8)	−0.0044 (5)	−0.0082 (6)	−0.0031 (5)
C2A	0.0177 (13)	0.0121 (13)	0.0149 (18)	0.0006 (9)	−0.0009 (12)	0.0091 (11)
C3A	0.0230 (14)	0.0157 (13)	0.0190 (17)	0.0003 (10)	0.0006 (12)	0.0047 (12)
C2B	0.0283 (19)	0.0254 (19)	0.020 (3)	−0.0005 (14)	−0.0019 (18)	0.0150 (17)
C3B	0.0280 (19)	0.0146 (17)	0.034 (3)	0.0035 (13)	−0.0072 (16)	−0.0028 (17)

C4	0.0255 (8)	0.0173 (8)	0.0509 (11)	−0.0012 (6)	−0.0064 (7)	−0.0047 (7)
C5	0.0228 (7)	0.0153 (7)	0.0197 (7)	−0.0009 (5)	0.0034 (5)	−0.0008 (5)
C6	0.0224 (7)	0.0191 (7)	0.0184 (7)	−0.0041 (5)	0.0044 (5)	−0.0012 (5)
C7	0.0197 (7)	0.0230 (7)	0.0161 (6)	0.0000 (6)	0.0045 (5)	0.0002 (5)
C8	0.0241 (7)	0.0171 (7)	0.0189 (7)	0.0030 (5)	0.0048 (5)	0.0004 (5)
C9	0.0229 (7)	0.0152 (7)	0.0221 (7)	−0.0029 (5)	0.0039 (6)	−0.0016 (5)
C10	0.0193 (7)	0.0181 (7)	0.0178 (6)	−0.0007 (5)	0.0033 (5)	−0.0007 (5)
C11	0.0206 (7)	0.0277 (8)	0.0246 (7)	0.0016 (6)	0.0050 (6)	0.0005 (6)
C12	0.0187 (7)	0.0156 (7)	0.0503 (10)	0.0005 (6)	0.0020 (7)	0.0060 (7)
C13	0.0300 (8)	0.0160 (7)	0.0223 (7)	0.0012 (6)	0.0017 (6)	0.0017 (6)
C14	0.0267 (7)	0.0158 (7)	0.0232 (7)	0.0003 (6)	0.0109 (6)	0.0005 (5)
C15	0.0195 (7)	0.0139 (6)	0.0234 (7)	0.0008 (5)	0.0046 (5)	−0.0024 (5)
C16	0.0285 (8)	0.0165 (7)	0.0222 (7)	0.0038 (6)	0.0084 (6)	0.0033 (5)
C17	0.0262 (8)	0.0173 (7)	0.0474 (10)	0.0022 (6)	0.0179 (7)	0.0092 (7)
C18	0.0203 (8)	0.0405 (11)	0.0943 (17)	−0.0063 (8)	0.0081 (9)	0.0218 (11)
O51	0.0198 (5)	0.0169 (5)	0.0252 (5)	−0.0019 (4)	0.0038 (4)	0.0021 (4)
O52	0.0236 (5)	0.0305 (6)	0.0253 (5)	−0.0017 (4)	0.0039 (4)	−0.0016 (5)
O54	0.0287 (5)	0.0185 (5)	0.0310 (6)	−0.0066 (4)	0.0094 (4)	−0.0016 (4)
C52A	0.0223 (8)	0.0175 (7)	0.0214 (8)	0.0015 (6)	0.0084 (6)	0.0010 (6)
C53A	0.0241 (8)	0.0157 (7)	0.0229 (8)	0.0005 (6)	0.0065 (6)	0.0009 (6)
C52B	0.0223 (8)	0.0175 (7)	0.0214 (8)	0.0015 (6)	0.0084 (6)	0.0010 (6)
C53B	0.0241 (8)	0.0157 (7)	0.0229 (8)	0.0005 (6)	0.0065 (6)	0.0009 (6)
C54	0.0259 (7)	0.0195 (7)	0.0206 (7)	−0.0039 (6)	0.0092 (6)	−0.0010 (6)
C55	0.0226 (7)	0.0186 (7)	0.0207 (7)	−0.0019 (5)	0.0093 (6)	−0.0028 (5)
C56	0.0222 (7)	0.0211 (7)	0.0234 (7)	−0.0046 (6)	0.0098 (6)	−0.0059 (6)
C57	0.0209 (7)	0.0253 (7)	0.0212 (7)	0.0001 (6)	0.0067 (6)	−0.0047 (6)
C58	0.0250 (7)	0.0207 (7)	0.0255 (7)	0.0027 (6)	0.0065 (6)	0.0005 (6)
C59	0.0244 (7)	0.0183 (7)	0.0275 (7)	−0.0025 (6)	0.0068 (6)	−0.0002 (6)
C60	0.0195 (7)	0.0200 (7)	0.0201 (7)	−0.0013 (5)	0.0062 (5)	−0.0023 (5)
C61	0.0211 (7)	0.0301 (8)	0.0303 (8)	0.0008 (6)	0.0051 (6)	−0.0051 (7)
C62	0.0220 (7)	0.0173 (7)	0.0305 (8)	0.0001 (6)	0.0051 (6)	0.0054 (6)
C63	0.0282 (8)	0.0250 (8)	0.0281 (8)	0.0003 (6)	0.0044 (6)	−0.0055 (6)
C64	0.0230 (7)	0.0251 (8)	0.0300 (8)	0.0034 (6)	0.0078 (6)	−0.0038 (6)
C65	0.0216 (7)	0.0184 (7)	0.0234 (7)	−0.0011 (5)	0.0056 (6)	0.0038 (6)
C66	0.0311 (8)	0.0215 (7)	0.0261 (7)	−0.0013 (6)	0.0128 (6)	−0.0006 (6)
C67	0.0267 (8)	0.0187 (7)	0.0359 (8)	0.0022 (6)	0.0145 (6)	0.0027 (6)
C68	0.0199 (7)	0.0384 (9)	0.0311 (8)	0.0007 (6)	0.0045 (6)	0.0058 (7)

Geometric parameters (Å, º)

O1—C10	1.3702 (16)	O51—C60	1.3679 (16)
O1—C2B	1.434 (2)	O51—C52B	1.474 (5)
O1—C2A	1.436 (2)	O51—C52A	1.4753 (17)
O2—C15	1.3643 (17)	O52—C65	1.3687 (17)
O2—C18	1.432 (2)	O52—C68	1.4302 (19)
O4—C4	1.2166 (19)	O54—C54	1.2224 (17)
C2A—C3A	1.535 (5)	C52A—C62	1.508 (2)
C2A—C12	1.561 (3)	C52A—C53A	1.516 (2)

C2A—H2A	1.0000	C52A—H52A	1.0000
C3A—C4	1.548 (2)	C53A—C54	1.520 (2)
C3A—H3A	0.9900	C53A—H53A	0.9900
C3A—H3B	0.9900	C53A—H53B	0.9900
C2B—C3B	1.484 (8)	C52B—C62	1.522 (5)
C2B—C12	1.513 (4)	C52B—C53B	1.55 (3)
C2B—H2B	1.0000	C52B—H52B	1.0000
C3B—C4	1.551 (2)	C53B—C54	1.517 (5)
C3B—H3C	0.9900	C53B—H53C	0.9900
C3B—H3D	0.9900	C53B—H53D	0.9900
C4—C5	1.473 (2)	C54—C55	1.479 (2)
C5—C10	1.4012 (19)	C55—C56	1.401 (2)
C5—C6	1.4015 (19)	C55—C60	1.4026 (19)
C6—C7	1.384 (2)	C56—C57	1.385 (2)
C6—H6	0.9500	C56—H56	0.9500
C7—C8	1.406 (2)	C57—C58	1.402 (2)
C7—C11	1.5082 (19)	C57—C61	1.5125 (19)
C8—C9	1.3829 (19)	C58—C59	1.382 (2)
C8—H8	0.9500	C58—H58	0.9500
C9—C10	1.3945 (19)	C59—C60	1.396 (2)
C9—H9	0.9500	C59—H59	0.9500
C11—H11A	0.9800	C61—H61A	0.9800
C11—H11B	0.9800	C61—H61B	0.9800
C11—H11C	0.9800	C61—H61C	0.9800
C12—C13	1.384 (2)	C62—C63	1.390 (2)
C12—C17	1.393 (2)	C62—C67	1.393 (2)
C13—C14	1.387 (2)	C63—C64	1.397 (2)
C13—H13	0.9500	C63—H63	0.9500
C14—C15	1.389 (2)	C64—C65	1.384 (2)
C14—H14	0.9500	C64—H64	0.9500
C15—C16	1.390 (2)	C65—C66	1.395 (2)
C16—C17	1.378 (2)	C66—C67	1.376 (2)
C16—H16	0.9500	C66—H66	0.9500
C17—H17	0.9500	C67—H67	0.9500
C18—H18A	0.9800	C68—H68A	0.9800
C18—H18B	0.9800	C68—H68B	0.9800
C18—H18C	0.9800	C68—H68C	0.9800

C10—O1—C2B	116.93 (19)	C60—O51—C52B	122.2 (6)
C10—O1—C2A	115.25 (15)	C60—O51—C52A	113.03 (10)
C15—O2—C18	117.06 (13)	C65—O52—C68	116.83 (12)
O1—C2A—C3A	113.1 (3)	O51—C52A—C62	107.21 (11)
O1—C2A—C12	104.68 (18)	O51—C52A—C53A	109.16 (12)
C3A—C2A—C12	110.1 (3)	C62—C52A—C53A	115.72 (13)
O1—C2A—H2A	109.6	O51—C52A—H52A	108.2
C3A—C2A—H2A	109.6	C62—C52A—H52A	108.2
C12—C2A—H2A	109.6	C53A—C52A—H52A	108.2
C2A—C3A—C4	104.6 (2)	C52A—C53A—C54	110.00 (13)

C2A—C3A—H3A	110.8	C52A—C53A—H53A	109.7
C4—C3A—H3A	110.8	C54—C53A—H53A	109.7
C2A—C3A—H3B	110.8	C52A—C53A—H53B	109.7
C4—C3A—H3B	110.8	C54—C53A—H53B	109.7
H3A—C3A—H3B	108.9	H53A—C53A—H53B	108.2
O1—C2B—C3B	111.1 (4)	O51—C52B—C62	106.6 (4)
O1—C2B—C12	107.3 (2)	O51—C52B—C53B	103.0 (15)
C3B—C2B—C12	112.4 (4)	C62—C52B—C53B	110.1 (13)
O1—C2B—H2B	108.6	O51—C52B—H52B	112.2
C3B—C2B—H2B	108.6	C62—C52B—H52B	112.2
C12—C2B—H2B	108.6	C53B—C52B—H52B	112.2
C2B—C3B—C4	109.6 (3)	C54—C53B—C52B	112.1 (13)
C2B—C3B—H3C	109.7	C54—C53B—H53C	109.2
C4—C3B—H3C	109.7	C52B—C53B—H53C	109.2
C2B—C3B—H3D	109.7	C54—C53B—H53D	109.2
C4—C3B—H3D	109.7	C52B—C53B—H53D	109.2
H3C—C3B—H3D	108.2	H53C—C53B—H53D	107.9
O4—C4—C5	123.46 (14)	O54—C54—C55	122.38 (13)
O4—C4—C3A	120.06 (17)	O54—C54—C53B	127.8 (8)
C5—C4—C3A	114.48 (15)	C55—C54—C53B	104.3 (9)
O4—C4—C3B	122.49 (19)	O54—C54—C53A	121.73 (13)
C5—C4—C3B	111.74 (18)	C55—C54—C53A	115.73 (12)
C10—C5—C6	119.21 (13)	C56—C55—C60	119.06 (13)
C10—C5—C4	119.99 (13)	C56—C55—C54	121.13 (13)
C6—C5—C4	120.76 (13)	C60—C55—C54	119.61 (12)
C7—C6—C5	121.68 (13)	C57—C56—C55	121.95 (13)
C7—C6—H6	119.2	C57—C56—H56	119.0
C5—C6—H6	119.2	C55—C56—H56	119.0
C6—C7—C8	117.72 (12)	C56—C57—C58	117.47 (13)
C6—C7—C11	121.96 (13)	C56—C57—C61	121.09 (13)
C8—C7—C11	120.32 (13)	C58—C57—C61	121.42 (14)
C9—C8—C7	121.96 (13)	C59—C58—C57	122.08 (14)
C9—C8—H8	119.0	C59—C58—H58	119.0
C7—C8—H8	119.0	C57—C58—H58	119.0
C8—C9—C10	119.43 (13)	C58—C59—C60	119.58 (13)
C8—C9—H9	120.3	C58—C59—H59	120.2
C10—C9—H9	120.3	C60—C59—H59	120.2
O1—C10—C9	117.06 (12)	O51—C60—C59	118.02 (12)
O1—C10—C5	122.94 (12)	O51—C60—C55	122.26 (13)
C9—C10—C5	119.99 (13)	C59—C60—C55	119.71 (13)
C7—C11—H11A	109.5	C57—C61—H61A	109.5
C7—C11—H11B	109.5	C57—C61—H61B	109.5
H11A—C11—H11B	109.5	H61A—C61—H61B	109.5
C7—C11—H11C	109.5	C57—C61—H61C	109.5
H11A—C11—H11C	109.5	H61A—C61—H61C	109.5
H11B—C11—H11C	109.5	H61B—C61—H61C	109.5
C13—C12—C17	118.41 (14)	C63—C62—C67	118.35 (14)
C13—C12—C2B	132.0 (2)	C63—C62—C52A	123.46 (14)

C17—C12—C2B	108.5 (2)	C67—C62—C52A	118.19 (14)
C13—C12—C2A	112.6 (2)	C63—C62—C52B	95.4 (8)
C17—C12—C2A	128.6 (2)	C67—C62—C52B	144.9 (6)
C12—C13—C14	121.40 (14)	C62—C63—C64	121.16 (14)
C12—C13—H13	119.3	C62—C63—H63	119.4
C14—C13—H13	119.3	C64—C63—H63	119.4
C13—C14—C15	119.30 (13)	C65—C64—C63	119.29 (14)
C13—C14—H14	120.4	C65—C64—H64	120.4
C15—C14—H14	120.4	C63—C64—H64	120.4
O2—C15—C14	124.98 (13)	O52—C65—C64	124.63 (13)
O2—C15—C16	115.02 (13)	O52—C65—C66	115.27 (13)
C14—C15—C16	120.00 (13)	C64—C65—C66	120.10 (13)
C17—C16—C15	119.83 (13)	C67—C66—C65	119.86 (14)
C17—C16—H16	120.1	C67—C66—H66	120.1
C15—C16—H16	120.1	C65—C66—H66	120.1
C16—C17—C12	121.06 (14)	C66—C67—C62	121.23 (14)
C16—C17—H17	119.5	C66—C67—H67	119.4
C12—C17—H17	119.5	C62—C67—H67	119.4
O2—C18—H18A	109.5	O52—C68—H68A	109.5
O2—C18—H18B	109.5	O52—C68—H68B	109.5
H18A—C18—H18B	109.5	H68A—C68—H68B	109.5
O2—C18—H18C	109.5	O52—C68—H68C	109.5
H18A—C18—H18C	109.5	H68A—C68—H68C	109.5
H18B—C18—H18C	109.5	H68B—C68—H68C	109.5

C10—O1—C2A—C3A	48.5 (4)	C60—O51—C52A—C62	−175.14 (12)
C10—O1—C2A—C12	168.42 (17)	C60—O51—C52A—C53A	58.80 (16)
O1—C2A—C3A—C4	−62.1 (4)	O51—C52A—C53A—C54	−58.34 (17)
C12—C2A—C3A—C4	−178.89 (19)	C62—C52A—C53A—C54	−179.35 (13)
C10—O1—C2B—C3B	−46.2 (6)	C60—O51—C52B—C62	−148.9 (8)
C10—O1—C2B—C12	−169.5 (3)	C60—O51—C52B—C53B	−32.9 (14)
O1—C2B—C3B—C4	60.1 (6)	O51—C52B—C53B—C54	63.6 (18)
C12—C2B—C3B—C4	−179.6 (2)	C62—C52B—C53B—C54	177.0 (12)
C2A—C3A—C4—O4	−151.0 (3)	C52B—C53B—C54—O54	141.1 (10)
C2A—C3A—C4—C5	44.6 (3)	C52B—C53B—C54—C55	−65.1 (17)
C2B—C3B—C4—O4	151.4 (3)	C52A—C53A—C54—O54	−157.54 (14)
C2B—C3B—C4—C5	−45.3 (5)	C52A—C53A—C54—C55	26.82 (19)
O4—C4—C5—C10	−179.48 (18)	O54—C54—C55—C56	5.2 (2)
C3A—C4—C5—C10	−15.6 (3)	C53B—C54—C55—C56	−150.5 (11)
C3B—C4—C5—C10	17.4 (3)	C53A—C54—C55—C56	−179.22 (14)
O4—C4—C5—C6	−2.0 (3)	O54—C54—C55—C60	−169.63 (14)
C3A—C4—C5—C6	161.8 (2)	C53B—C54—C55—C60	34.8 (11)
C3B—C4—C5—C6	−165.1 (3)	C53A—C54—C55—C60	6.0 (2)
C10—C5—C6—C7	0.6 (2)	C60—C55—C56—C57	1.1 (2)
C4—C5—C6—C7	−176.88 (15)	C54—C55—C56—C57	−173.69 (13)
C5—C6—C7—C8	0.6 (2)	C55—C56—C57—C58	2.3 (2)
C5—C6—C7—C11	−179.56 (13)	C55—C56—C57—C61	−176.36 (13)
C6—C7—C8—C9	−1.3 (2)	C56—C57—C58—C59	−3.1 (2)

C11—C7—C8—C9	178.87 (13)	C61—C57—C58—C59	175.51 (14)
C7—C8—C9—C10	0.7 (2)	C57—C58—C59—C60	0.5 (2)
C2B—O1—C10—C9	−162.0 (3)	C52B—O51—C60—C59	−171.6 (10)
C2A—O1—C10—C9	167.3 (2)	C52A—O51—C60—C59	155.67 (13)
C2B—O1—C10—C5	16.7 (4)	C52B—O51—C60—C55	7.2 (11)
C2A—O1—C10—C5	−14.0 (3)	C52A—O51—C60—C55	−25.51 (18)
C8—C9—C10—O1	179.31 (12)	C58—C59—C60—O51	−178.12 (13)
C8—C9—C10—C5	0.5 (2)	C58—C59—C60—C55	3.0 (2)
C6—C5—C10—O1	−179.89 (13)	C56—C55—C60—O51	177.38 (13)
C4—C5—C10—O1	−2.4 (2)	C54—C55—C60—O51	−7.7 (2)
C6—C5—C10—C9	−1.2 (2)	C56—C55—C60—C59	−3.8 (2)
C4—C5—C10—C9	176.34 (15)	C54—C55—C60—C59	171.09 (13)
O1—C2B—C12—C13	25.7 (6)	O51—C52A—C62—C63	−88.39 (17)
C3B—C2B—C12—C13	−96.8 (3)	C53A—C52A—C62—C63	33.7 (2)
O1—C2B—C12—C17	−142.1 (3)	O51—C52A—C62—C67	90.90 (16)
C3B—C2B—C12—C17	95.5 (5)	C53A—C52A—C62—C67	−147.06 (15)
O1—C2A—C12—C13	73.8 (3)	O51—C52B—C62—C63	−127.5 (13)
C3A—C2A—C12—C13	−164.3 (3)	C53B—C52B—C62—C63	121.4 (13)
O1—C2A—C12—C17	−113.9 (2)	O51—C52B—C62—C67	37 (2)
C3A—C2A—C12—C17	8.0 (4)	C53B—C52B—C62—C67	−74.3 (13)
C17—C12—C13—C14	0.2 (2)	C67—C62—C63—C64	−0.5 (2)
C2B—C12—C13—C14	−166.6 (4)	C52A—C62—C63—C64	178.76 (14)
C2A—C12—C13—C14	173.36 (15)	C52B—C62—C63—C64	169.3 (6)
C12—C13—C14—C15	0.3 (2)	C62—C63—C64—C65	0.0 (2)
C18—O2—C15—C14	0.9 (2)	C68—O52—C65—C64	2.6 (2)
C18—O2—C15—C16	−179.18 (16)	C68—O52—C65—C66	−177.58 (13)
C13—C14—C15—O2	179.35 (13)	C63—C64—C65—O52	−179.56 (14)
C13—C14—C15—C16	−0.6 (2)	C63—C64—C65—C66	0.6 (2)
O2—C15—C16—C17	−179.48 (13)	O52—C65—C66—C67	179.44 (13)
C14—C15—C16—C17	0.5 (2)	C64—C65—C66—C67	−0.7 (2)
C15—C16—C17—C12	0.0 (2)	C65—C66—C67—C62	0.2 (2)
C13—C12—C17—C16	−0.3 (2)	C63—C62—C67—C66	0.4 (2)
C2B—C12—C17—C16	169.3 (3)	C52A—C62—C67—C66	−178.90 (14)
C2A—C12—C17—C16	−172.25 (19)	C52B—C62—C67—C66	−161.8 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O4^{i}	0.95	2.55	3.231 (2)	129
C16—H16···O1^{ii}	0.95	2.51	3.415 (2)	160
C52*A*—H52*A*···O54^{iii}	1.00	2.35	3.216 (2)	145
C68—H68*B*···O4^{iv}	0.98	2.46	3.330 (2)	147

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iv) −*x*+2, −*y*+1, −*z*+1.

2-(4-Chlorophenyl)-3,4-dihydro-2*H*-1-benzopyran-4-one (FL5)

Crystal data

$C_{15}H_{11}ClO_2$
$M_r = 258.69$
Monoclinic, $P2_1/c$
$a = 6.4760$ (2) Å
$b = 16.2902$ (4) Å
$c = 11.6755$ (4) Å
$\beta = 97.953$ (3)°
$V = 1219.86$ (6) Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.409$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4722 reflections
$\theta = 3.4$–33.0°
$\mu = 0.30$ mm^{-1}
$T = 100$ K
Prism, colourless
0.3 × 0.2 × 0.1 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: micro-focus sealed X-ray tube, SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4498 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
$T_{min} = 0.801$, $T_{max} = 1.000$
16927 measured reflections
2525 independent reflections
2414 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 26.5°$, $\theta_{min} = 3.1°$
$h = -5\rightarrow8$
$k = -20\rightarrow20$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.073$
$S = 1.06$
2525 reflections
163 parameters
0 restraints
Primary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.6483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray data of five flavanone derivatives (**FL1**, **FL2**, **FL3**, **FL5** and **FL8**) were collected on a micro-focus SuperNova diffractometer with an Atlas detector, whereas data collection of two chalcone derivatives (**CH2** and **CH4**) was carried out on an Xcalibur diffractometer with a Sapphire3 detector; all using Mo $K\alpha$ and ω scans at a low temperature of 100.0 (1) K. The X-ray data were corrected for absorption using *CrysAlis PRO* (Agilent, 2015). All structures were solved using SHELXT (Sheldrick, 2015a) and refined with SHELXL2014/7 (Sheldrick, 2015b). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.20419 (4)	0.46628 (2)	0.17410 (3)	0.01972 (10)
O1	0.54812 (12)	0.63334 (5)	0.50329 (7)	0.01536 (18)
O4	0.45832 (13)	0.88173 (5)	0.44105 (7)	0.01890 (19)

C2	0.57080 (17)	0.66607 (7)	0.38888 (9)	0.0145 (2)
H2	0.4333	0.6619	0.3383	0.017*
C3	0.63526 (18)	0.75684 (7)	0.39913 (10)	0.0166 (2)
H3A	0.7740	0.7615	0.4464	0.020*
H3B	0.6463	0.7790	0.3212	0.020*
C4	0.47772 (17)	0.80718 (7)	0.45450 (9)	0.0144 (2)
C5	0.35693 (17)	0.75952 (7)	0.53160 (9)	0.0137 (2)
C6	0.20372 (17)	0.79870 (7)	0.58686 (10)	0.0160 (2)
H6	0.1655	0.8538	0.5678	0.019*
C7	0.10829 (18)	0.75693 (7)	0.66924 (10)	0.0175 (2)
H7	0.0031	0.7830	0.7054	0.021*
C8	0.16879 (18)	0.67552 (7)	0.69884 (10)	0.0171 (2)
H8	0.1070	0.6479	0.7572	0.021*
C9	0.31722 (18)	0.63490 (7)	0.64420 (10)	0.0158 (2)
H9	0.3564	0.5801	0.6647	0.019*
C10	0.40800 (17)	0.67644 (7)	0.55821 (9)	0.0132 (2)
C12	0.72741 (18)	0.61290 (7)	0.33822 (10)	0.0146 (2)
C13	0.92054 (18)	0.59337 (7)	0.40307 (10)	0.0165 (2)
H13	0.9513	0.6115	0.4809	0.020*
C14	1.06753 (18)	0.54741 (7)	0.35354 (10)	0.0165 (2)
H14	1.1976	0.5334	0.3972	0.020*
C15	1.01883 (18)	0.52229 (7)	0.23770 (10)	0.0149 (2)
C16	0.82736 (18)	0.54032 (7)	0.17183 (10)	0.0157 (2)
H16	0.7969	0.5222	0.0940	0.019*
C17	0.68179 (17)	0.58561 (7)	0.22317 (10)	0.0152 (2)
H17	0.5504	0.5982	0.1799	0.018*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.01935 (16)	0.01612 (16)	0.02614 (17)	0.00188 (10)	0.01179 (12)	−0.00180 (11)
O1	0.0178 (4)	0.0142 (4)	0.0154 (4)	0.0032 (3)	0.0071 (3)	0.0027 (3)
O4	0.0244 (4)	0.0128 (4)	0.0206 (4)	0.0001 (3)	0.0071 (3)	0.0015 (3)
C2	0.0150 (5)	0.0154 (5)	0.0135 (5)	0.0000 (4)	0.0035 (4)	0.0014 (4)
C3	0.0182 (5)	0.0142 (5)	0.0188 (5)	0.0000 (4)	0.0076 (4)	0.0023 (4)
C4	0.0151 (5)	0.0149 (5)	0.0131 (5)	−0.0008 (4)	0.0014 (4)	−0.0005 (4)
C5	0.0143 (5)	0.0139 (5)	0.0128 (5)	−0.0016 (4)	0.0019 (4)	−0.0013 (4)
C6	0.0167 (5)	0.0139 (5)	0.0176 (5)	−0.0002 (4)	0.0027 (4)	−0.0021 (4)
C7	0.0154 (5)	0.0196 (6)	0.0186 (5)	−0.0011 (4)	0.0062 (4)	−0.0050 (4)
C8	0.0175 (5)	0.0202 (6)	0.0144 (5)	−0.0045 (4)	0.0048 (4)	−0.0004 (4)
C9	0.0175 (5)	0.0146 (5)	0.0154 (5)	−0.0014 (4)	0.0029 (4)	0.0013 (4)
C10	0.0119 (5)	0.0148 (5)	0.0127 (5)	−0.0007 (4)	0.0010 (4)	−0.0015 (4)
C12	0.0160 (5)	0.0112 (5)	0.0175 (5)	−0.0014 (4)	0.0062 (4)	0.0016 (4)
C13	0.0195 (6)	0.0167 (5)	0.0135 (5)	−0.0019 (4)	0.0035 (4)	−0.0010 (4)
C14	0.0136 (5)	0.0163 (5)	0.0194 (6)	−0.0009 (4)	0.0017 (4)	0.0024 (4)
C15	0.0163 (5)	0.0099 (5)	0.0203 (6)	−0.0009 (4)	0.0092 (4)	0.0005 (4)
C16	0.0191 (6)	0.0136 (5)	0.0149 (5)	−0.0033 (4)	0.0044 (4)	−0.0009 (4)
C17	0.0139 (5)	0.0141 (5)	0.0175 (5)	−0.0012 (4)	0.0024 (4)	0.0024 (4)

Geometric parameters (Å, º)

Cl1—C15	1.7526 (11)	C7—H7	0.9500
O1—C10	1.3743 (13)	C8—C9	1.3923 (16)
O1—C2	1.4644 (13)	C8—H8	0.9500
O4—C4	1.2288 (14)	C9—C10	1.4053 (16)
C2—C12	1.5148 (15)	C9—H9	0.9500
C2—C3	1.5367 (16)	C12—C13	1.4060 (16)
C2—H2	1.0000	C12—C17	1.4069 (16)
C3—C4	1.5212 (15)	C13—C14	1.3977 (16)
C3—H3A	0.9900	C13—H13	0.9500
C3—H3B	0.9900	C14—C15	1.4064 (16)
C4—C5	1.4899 (15)	C14—H14	0.9500
C5—C6	1.4090 (16)	C15—C16	1.3969 (17)
C5—C10	1.4174 (16)	C16—C17	1.3960 (16)
C6—C7	1.3908 (16)	C16—H16	0.9500
C6—H6	0.9500	C17—H17	0.9500
C7—C8	1.4121 (17)		
C10—O1—C2	113.30 (8)	C9—C8—H8	119.3
O1—C2—C12	107.76 (9)	C7—C8—H8	119.3
O1—C2—C3	109.86 (9)	C8—C9—C10	118.82 (11)
C12—C2—C3	113.03 (9)	C8—C9—H9	120.6
O1—C2—H2	108.7	C10—C9—H9	120.6
C12—C2—H2	108.7	O1—C10—C9	117.12 (10)
C3—C2—H2	108.7	O1—C10—C5	122.32 (10)
C4—C3—C2	111.15 (9)	C9—C10—C5	120.56 (10)
C4—C3—H3A	109.4	C13—C12—C17	119.75 (10)
C2—C3—H3A	109.4	C13—C12—C2	120.85 (10)
C4—C3—H3B	109.4	C17—C12—C2	119.34 (10)
C2—C3—H3B	109.4	C14—C13—C12	120.29 (10)
H3A—C3—H3B	108.0	C14—C13—H13	119.9
O4—C4—C5	122.64 (10)	C12—C13—H13	119.9
O4—C4—C3	122.77 (10)	C13—C14—C15	118.61 (10)
C5—C4—C3	114.52 (10)	C13—C14—H14	120.7
C6—C5—C10	119.33 (10)	C15—C14—H14	120.7
C6—C5—C4	120.16 (10)	C16—C15—C14	122.15 (10)
C10—C5—C4	120.26 (10)	C16—C15—Cl1	118.95 (9)
C7—C6—C5	120.23 (11)	C14—C15—Cl1	118.90 (9)
C7—C6—H6	119.9	C17—C16—C15	118.39 (10)
C5—C6—H6	119.9	C17—C16—H16	120.8
C6—C7—C8	119.60 (10)	C15—C16—H16	120.8
C6—C7—H7	120.2	C16—C17—C12	120.79 (10)
C8—C7—H7	120.2	C16—C17—H17	119.6
C9—C8—C7	121.33 (10)	C12—C17—H17	119.6
C10—O1—C2—C12	−179.63 (9)	C6—C5—C10—O1	176.64 (10)
C10—O1—C2—C3	56.83 (11)	C4—C5—C10—O1	−9.05 (16)

O1—C2—C3—C4	−57.46 (12)	C6—C5—C10—C9	−4.14 (16)
C12—C2—C3—C4	−177.86 (9)	C4—C5—C10—C9	170.18 (10)
C2—C3—C4—O4	−157.39 (11)	O1—C2—C12—C13	−49.03 (13)
C2—C3—C4—C5	25.82 (13)	C3—C2—C12—C13	72.56 (13)
O4—C4—C5—C6	4.15 (17)	O1—C2—C12—C17	133.56 (10)
C3—C4—C5—C6	−179.05 (10)	C3—C2—C12—C17	−104.85 (12)
O4—C4—C5—C10	−170.11 (11)	C17—C12—C13—C14	0.34 (17)
C3—C4—C5—C10	6.69 (15)	C2—C12—C13—C14	−177.06 (10)
C10—C5—C6—C7	1.94 (16)	C12—C13—C14—C15	0.80 (17)
C4—C5—C6—C7	−172.38 (10)	C13—C14—C15—C16	−1.38 (17)
C5—C6—C7—C8	1.24 (17)	C13—C14—C15—Cl1	178.82 (8)
C6—C7—C8—C9	−2.34 (17)	C14—C15—C16—C17	0.77 (17)
C7—C8—C9—C10	0.17 (17)	Cl1—C15—C16—C17	−179.43 (8)
C2—O1—C10—C9	156.80 (10)	C15—C16—C17—C12	0.42 (16)
C2—O1—C10—C5	−23.95 (14)	C13—C12—C17—C16	−0.97 (17)
C8—C9—C10—O1	−177.67 (9)	C2—C12—C17—C16	176.47 (10)
C8—C9—C10—C5	3.07 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—Cl1···O4^{i}	1.75	3.05 (1)	4.798 (2)	175

Symmetry code: (i) −*x*+2, *y*−1/2, −*z*+1/2.

8-Bromo-6-methyl-2-phenyl-3,4-dihydro-2*H*-1-benzopyran-4-one (FL8)

Crystal data

$C_{16}H_{13}BrO_2$
M_r = 317.17
Monoclinic, $P2_1/n$
a = 15.2121 (7) Å
b = 8.7614 (2) Å
c = 20.7260 (6) Å
β = 92.458 (3)°
V = 2759.81 (16) Å^3
Z = 8

$F(000)$ = 1280
D_x = 1.527 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 11075 reflections
θ = 3.3–39.1°
μ = 2.97 mm^{-1}
T = 100 K
Prism, colourless
0.2 × 0.1 × 0.1 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Mirror monochromator
Detector resolution: 10.4498 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.524, T_{max} = 1.000

30046 measured reflections
5682 independent reflections
4561 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 26.5°, θ_{min} = 2.9°
h = −19→19
k = −8→11
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.095$
$S = 1.05$
5682 reflections
351 parameters
6 restraints

Primary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0254P)^2 + 3.6602P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.98$ e Å^{-3}
$\Delta\rho_{min} = -0.61$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray data of five flavanone derivatives (**FL1**, **FL2**, **FL3**, **FL5** and **FL8**) were collected on a micro-focus SuperNova diffractometer with an Atlas detector, whereas data collection of two chalcone derivatives (**CH2** and **CH4**) was carried out on an Xcalibur diffractometer with a Sapphire3 detector; all using Mo *Kα* and *ω* scans at a low temperature of 100.0 (1) K. The X-ray data were corrected for absorption using *CrysAlis PRO* (Agilent, 2015). All structures were solved using SHELXT (Sheldrick, 2015a) and refined with SHELXL2014/7 (Sheldrick, 2015b). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.10490 (2)	0.35851 (4)	−0.03593 (2)	0.02302 (10)	
O1	0.12423 (15)	0.6946 (2)	−0.02408 (11)	0.0203 (5)	
O4	0.21704 (18)	0.9584 (3)	0.12826 (12)	0.0325 (6)	
C2A	0.1526 (3)	0.8513 (4)	−0.03329 (19)	0.0250 (10)	0.928 (7)
H2A	0.2174	0.8509	−0.0397	0.030*	0.928 (7)
C2B	0.0922 (7)	0.8509 (7)	−0.0271 (3)	0.0250 (10)	0.072 (7)
H2B	0.0274	0.8494	−0.0205	0.030*	0.072 (7)
C3	0.1356 (3)	0.9446 (4)	0.02593 (18)	0.0352 (10)	
H3A	0.0717	0.9462	0.0330	0.042*	0.928 (7)
H3B	0.1551	1.0509	0.0191	0.042*	0.928 (7)
H3C	0.0893	1.0122	0.0421	0.042*	0.072 (7)
H3D	0.1781	1.0118	0.0049	0.042*	0.072 (7)
C4	0.1838 (2)	0.8797 (4)	0.08504 (17)	0.0262 (8)	
C5	0.1848 (2)	0.7105 (4)	0.08718 (16)	0.0206 (7)	
C6	0.2153 (2)	0.6325 (4)	0.14264 (17)	0.0236 (7)	
H6	0.2375	0.6893	0.1788	0.028*	
C7	0.2142 (2)	0.4748 (4)	0.14611 (17)	0.0246 (8)	
C8	0.1805 (2)	0.3952 (4)	0.09186 (17)	0.0230 (7)	
H8	0.1791	0.2869	0.0929	0.028*	
C9	0.1492 (2)	0.4700 (4)	0.03698 (16)	0.0198 (7)	
C10	0.1520 (2)	0.6292 (4)	0.03300 (16)	0.0187 (7)	
C11	0.2476 (3)	0.3887 (4)	0.20639 (18)	0.0316 (9)	
H11A	0.2985	0.4425	0.2261	0.047*	
H11B	0.2651	0.2852	0.1944	0.047*	

H11C	0.2008	0.3832	0.2373	0.047*	
C12	0.1066 (2)	0.9125 (4)	−0.09402 (18)	0.0269 (8)	
C13	0.0252 (2)	0.8560 (4)	−0.11740 (18)	0.0282 (8)	
H13	−0.0024	0.7747	−0.0957	0.034*	
C14	−0.0148 (3)	0.9195 (4)	−0.17251 (19)	0.0328 (9)	
H14	−0.0698	0.8809	−0.1887	0.039*	
C15	0.0252 (3)	1.0397 (4)	−0.20416 (19)	0.0345 (9)	
H15	−0.0025	1.0830	−0.2418	0.041*	
C16	0.1058 (3)	1.0962 (4)	−0.18056 (19)	0.0334 (9)	
H16	0.1330	1.1787	−0.2018	0.040*	
C17	0.1463 (2)	1.0316 (4)	−0.12600 (19)	0.0300 (8)	
H17	0.2017	1.0692	−0.1103	0.036*	
Br51	0.45390 (2)	0.63182 (4)	0.14107 (2)	0.02582 (10)	
O51	0.45483 (15)	0.2913 (2)	0.12764 (11)	0.0237 (5)	
O54	0.35363 (18)	0.0195 (3)	−0.01903 (14)	0.0386 (7)	
C52A	0.4912 (3)	0.1394 (4)	0.1183 (2)	0.0285 (11)	0.814 (7)
H52A	0.5425	0.1486	0.0901	0.034*	0.814 (7)
C52B	0.4432 (6)	0.1313 (7)	0.1436 (4)	0.0285 (11)	0.186 (7)
H52B	0.3912	0.1231	0.1713	0.034*	0.186 (7)
C53	0.4256 (3)	0.0381 (5)	0.0861 (2)	0.0475 (12)	
H53A	0.3778	0.0187	0.1159	0.057*	0.814 (7)
H53B	0.4539	−0.0610	0.0772	0.057*	0.814 (7)
H53C	0.3866	−0.0459	0.0991	0.057*	0.186 (7)
H53D	0.4823	−0.0096	0.0756	0.057*	0.186 (7)
C54	0.3862 (2)	0.1013 (4)	0.0237 (2)	0.0329 (9)	
C55	0.3877 (2)	0.2694 (4)	0.01884 (17)	0.0234 (8)	
C56	0.3559 (2)	0.3434 (4)	−0.03726 (18)	0.0267 (8)	
H56	0.3352	0.2839	−0.0731	0.032*	
C57	0.3537 (2)	0.5005 (4)	−0.04204 (17)	0.0256 (8)	
C58	0.3827 (2)	0.5846 (4)	0.01242 (17)	0.0238 (8)	
H58	0.3802	0.6929	0.0109	0.029*	
C59	0.4149 (2)	0.5144 (4)	0.06800 (17)	0.0220 (7)	
C60	0.4197 (2)	0.3556 (4)	0.07230 (16)	0.0217 (7)	
C61	0.3225 (2)	0.5775 (4)	−0.10422 (18)	0.0319 (9)	
H61A	0.3722	0.5897	−0.1324	0.048*	
H61B	0.2981	0.6781	−0.0945	0.048*	
H61C	0.2770	0.5148	−0.1261	0.048*	
C62	0.5246 (3)	0.0814 (4)	0.1842 (2)	0.0427 (11)	
C63	0.4734 (3)	0.0766 (4)	0.2407 (2)	0.0390 (10)	
H63	0.4146	0.1133	0.2389	0.047*	
C64	0.5102 (3)	0.0180 (4)	0.2978 (2)	0.0348 (9)	
H64	0.4773	0.0150	0.3357	0.042*	
C65	0.5962 (2)	−0.0363 (4)	0.29866 (19)	0.0309 (9)	
H65	0.6218	−0.0772	0.3375	0.037*	
C66	0.6457 (3)	−0.0318 (5)	0.2434 (2)	0.0455 (11)	
H66	0.7042	−0.0702	0.2450	0.055*	
C67	0.6103 (3)	0.0279 (5)	0.1867 (2)	0.0500 (12)	
H67	0.6444	0.0323	0.1494	0.060*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0318 (2)	0.01882 (17)	0.01830 (19)	−0.00322 (13)	−0.00003 (13)	−0.00123 (13)
O1	0.0284 (13)	0.0174 (11)	0.0151 (13)	0.0001 (9)	0.0003 (9)	0.0000 (9)
O4	0.0478 (16)	0.0278 (13)	0.0215 (15)	−0.0042 (12)	−0.0022 (12)	−0.0075 (11)
C2A	0.031 (2)	0.0170 (18)	0.027 (2)	−0.0013 (15)	−0.0029 (16)	−0.0036 (16)
C2B	0.031 (2)	0.0170 (18)	0.027 (2)	−0.0013 (15)	−0.0029 (16)	−0.0036 (16)
C3	0.062 (3)	0.0211 (19)	0.022 (2)	0.0031 (18)	−0.0053 (18)	−0.0036 (16)
C4	0.034 (2)	0.0259 (19)	0.0187 (19)	0.0010 (15)	0.0027 (15)	−0.0058 (15)
C5	0.0242 (17)	0.0217 (17)	0.0161 (18)	0.0023 (13)	0.0024 (13)	−0.0024 (14)
C6	0.0247 (17)	0.0267 (18)	0.0192 (19)	0.0025 (14)	−0.0006 (13)	−0.0047 (15)
C7	0.0255 (18)	0.0300 (19)	0.0183 (19)	0.0044 (15)	0.0011 (14)	0.0006 (15)
C8	0.0262 (18)	0.0186 (16)	0.025 (2)	0.0021 (14)	0.0044 (14)	0.0032 (15)
C9	0.0232 (17)	0.0204 (16)	0.0161 (18)	0.0014 (13)	0.0046 (13)	−0.0041 (14)
C10	0.0206 (16)	0.0220 (16)	0.0139 (17)	0.0021 (13)	0.0034 (12)	0.0005 (14)
C11	0.038 (2)	0.038 (2)	0.018 (2)	0.0067 (17)	−0.0038 (15)	0.0013 (17)
C12	0.038 (2)	0.0194 (17)	0.023 (2)	0.0016 (15)	−0.0017 (15)	−0.0054 (15)
C13	0.040 (2)	0.0237 (18)	0.021 (2)	−0.0016 (15)	0.0020 (15)	−0.0004 (15)
C14	0.035 (2)	0.034 (2)	0.029 (2)	0.0016 (17)	−0.0055 (16)	−0.0006 (18)
C15	0.053 (3)	0.032 (2)	0.017 (2)	0.0031 (18)	−0.0041 (17)	0.0005 (17)
C16	0.050 (2)	0.0263 (19)	0.024 (2)	−0.0043 (17)	0.0039 (17)	0.0005 (16)
C17	0.036 (2)	0.0218 (18)	0.031 (2)	−0.0011 (15)	−0.0020 (16)	−0.0051 (16)
Br51	0.0314 (2)	0.02158 (18)	0.0242 (2)	0.00053 (14)	−0.00135 (14)	−0.00126 (15)
O51	0.0310 (13)	0.0189 (12)	0.0208 (14)	0.0009 (10)	−0.0016 (10)	0.0010 (10)
O54	0.0484 (17)	0.0310 (14)	0.0354 (18)	−0.0056 (12)	−0.0088 (13)	−0.0103 (13)
C52A	0.041 (3)	0.022 (2)	0.022 (3)	0.006 (2)	0.0052 (18)	−0.0015 (19)
C52B	0.041 (3)	0.022 (2)	0.022 (3)	0.006 (2)	0.0052 (18)	−0.0015 (19)
C53	0.060 (3)	0.027 (2)	0.052 (3)	−0.0001 (19)	−0.032 (2)	−0.001 (2)
C54	0.034 (2)	0.0276 (19)	0.037 (2)	−0.0003 (16)	−0.0037 (17)	−0.0038 (18)
C55	0.0222 (17)	0.0243 (18)	0.024 (2)	−0.0012 (14)	0.0030 (14)	−0.0012 (15)
C56	0.0231 (18)	0.034 (2)	0.023 (2)	−0.0043 (15)	0.0023 (14)	−0.0034 (16)
C57	0.0210 (18)	0.035 (2)	0.021 (2)	0.0010 (15)	0.0019 (14)	0.0042 (16)
C58	0.0217 (17)	0.0250 (18)	0.025 (2)	0.0016 (14)	0.0028 (14)	0.0035 (15)
C59	0.0206 (17)	0.0217 (17)	0.024 (2)	−0.0001 (13)	0.0031 (14)	−0.0016 (15)
C60	0.0221 (17)	0.0256 (18)	0.0177 (18)	0.0004 (14)	0.0037 (13)	0.0000 (15)
C61	0.030 (2)	0.037 (2)	0.028 (2)	0.0028 (16)	−0.0032 (16)	0.0064 (18)
C62	0.085 (3)	0.0183 (18)	0.024 (2)	0.001 (2)	−0.009 (2)	0.0014 (17)
C63	0.041 (2)	0.029 (2)	0.046 (3)	0.0042 (17)	−0.0088 (19)	0.0052 (19)
C64	0.037 (2)	0.041 (2)	0.026 (2)	−0.0038 (18)	0.0013 (16)	0.0064 (18)
C65	0.035 (2)	0.033 (2)	0.024 (2)	−0.0019 (16)	−0.0039 (16)	0.0066 (17)
C66	0.056 (3)	0.050 (3)	0.031 (3)	0.011 (2)	0.010 (2)	0.002 (2)
C67	0.082 (4)	0.040 (2)	0.029 (3)	0.013 (2)	0.014 (2)	0.001 (2)

Geometric parameters (Å, º)

Br1—C9	1.898 (3)	Br51—C59	1.904 (3)
O1—C10	1.365 (4)	O51—C60	1.366 (4)

O1—C2A	1.454 (4)	O51—C52B	1.454 (6)
O1—C2B	1.454 (6)	O51—C52A	1.458 (4)
O4—C4	1.222 (4)	O54—C54	1.227 (4)
C2A—C3	1.506 (5)	C52A—C53	1.473 (5)
C2A—C12	1.512 (5)	C52A—C62	1.523 (6)
C2A—H2A	1.0000	C52A—H52A	1.0000
C2B—C3	1.502 (7)	C52B—C53	1.460 (7)
C2B—C12	1.513 (7)	C52B—C62	1.530 (7)
C2B—H2B	1.0000	C52B—H52B	1.0000
C3—C4	1.511 (5)	C53—C54	1.508 (5)
C3—H3A	0.9900	C53—H53A	0.9900
C3—H3B	0.9900	C53—H53B	0.9900
C3—H3C	0.9900	C53—H53C	0.9900
C3—H3D	0.9900	C53—H53D	0.9900
C4—C5	1.483 (5)	C54—C55	1.477 (5)
C5—C6	1.400 (5)	C55—C56	1.400 (5)
C5—C10	1.403 (4)	C55—C60	1.411 (5)
C6—C7	1.384 (5)	C56—C57	1.380 (5)
C6—H6	0.9500	C56—H56	0.9500
C7—C8	1.401 (5)	C57—C58	1.404 (5)
C7—C11	1.528 (5)	C57—C61	1.513 (5)
C8—C9	1.379 (5)	C58—C59	1.377 (5)
C8—H8	0.9500	C58—H58	0.9500
C9—C10	1.398 (4)	C59—C60	1.396 (5)
C11—H11A	0.9800	C61—H61A	0.9800
C11—H11B	0.9800	C61—H61B	0.9800
C11—H11C	0.9800	C61—H61C	0.9800
C12—C17	1.388 (5)	C62—C67	1.384 (6)
C12—C13	1.400 (5)	C62—C63	1.434 (6)
C13—C14	1.388 (5)	C63—C64	1.387 (5)
C13—H13	0.9500	C63—H63	0.9500
C14—C15	1.395 (5)	C64—C65	1.391 (5)
C14—H14	0.9500	C64—H64	0.9500
C15—C16	1.391 (5)	C65—C66	1.399 (6)
C15—H15	0.9500	C65—H65	0.9500
C16—C17	1.385 (5)	C66—C67	1.375 (6)
C16—H16	0.9500	C66—H66	0.9500
C17—H17	0.9500	C67—H67	0.9500

C10—O1—C2A	115.3 (3)	C60—O51—C52B	122.9 (3)
C10—O1—C2B	121.6 (3)	C60—O51—C52A	113.7 (3)
O1—C2A—C3	110.1 (3)	O51—C52A—C53	110.9 (3)
O1—C2A—C12	108.4 (3)	O51—C52A—C62	107.5 (3)
C3—C2A—C12	113.4 (3)	C53—C52A—C62	113.5 (3)
O1—C2A—H2A	108.3	O51—C52A—H52A	108.3
C3—C2A—H2A	108.3	C53—C52A—H52A	108.3
C12—C2A—H2A	108.3	C62—C52A—H52A	108.3
O1—C2B—C3	110.3 (5)	O51—C52B—C53	111.9 (5)

O1—C2B—C12	108.3 (5)	O51—C52B—C62	107.3 (5)
C3—C2B—C12	113.5 (5)	C53—C52B—C62	113.9 (5)
O1—C2B—H2B	108.2	O51—C52B—H52B	107.8
C3—C2B—H2B	108.2	C53—C52B—H52B	107.8
C12—C2B—H2B	108.2	C62—C52B—H52B	107.8
C2B—C3—C4	124.8 (4)	C52B—C53—C54	123.2 (4)
C2A—C3—C4	111.2 (3)	C52A—C53—C54	113.9 (3)
C2A—C3—H3A	109.4	C52A—C53—H53A	108.8
C4—C3—H3A	109.4	C54—C53—H53A	108.8
C2A—C3—H3B	109.4	C52A—C53—H53B	108.8
C4—C3—H3B	109.4	C54—C53—H53B	108.8
H3A—C3—H3B	108.0	H53A—C53—H53B	107.7
C2B—C3—H3C	106.1	C52B—C53—H53C	106.5
C4—C3—H3C	106.1	C54—C53—H53C	106.5
C2B—C3—H3D	106.1	C52B—C53—H53D	106.5
C4—C3—H3D	106.1	C54—C53—H53D	106.5
H3C—C3—H3D	106.3	H53C—C53—H53D	106.5
O4—C4—C5	122.6 (3)	O54—C54—C55	122.7 (4)
O4—C4—C3	123.5 (3)	O54—C54—C53	122.6 (3)
C5—C4—C3	113.8 (3)	C55—C54—C53	114.7 (3)
C6—C5—C10	120.2 (3)	C56—C55—C60	120.0 (3)
C6—C5—C4	121.0 (3)	C56—C55—C54	120.9 (3)
C10—C5—C4	118.7 (3)	C60—C55—C54	119.1 (3)
C7—C6—C5	121.7 (3)	C57—C56—C55	121.9 (3)
C7—C6—H6	119.2	C57—C56—H56	119.1
C5—C6—H6	119.2	C55—C56—H56	119.1
C6—C7—C8	117.4 (3)	C56—C57—C58	117.4 (3)
C6—C7—C11	122.1 (3)	C56—C57—C61	120.8 (3)
C8—C7—C11	120.5 (3)	C58—C57—C61	121.8 (3)
C9—C8—C7	121.8 (3)	C59—C58—C57	121.8 (3)
C9—C8—H8	119.1	C59—C58—H58	119.1
C7—C8—H8	119.1	C57—C58—H58	119.1
C8—C9—C10	120.8 (3)	C58—C59—C60	120.9 (3)
C8—C9—Br1	120.7 (2)	C58—C59—Br51	120.8 (3)
C10—C9—Br1	118.5 (3)	C60—C59—Br51	118.3 (3)
O1—C10—C9	117.5 (3)	O51—C60—C59	118.8 (3)
O1—C10—C5	124.5 (3)	O51—C60—C55	123.2 (3)
C9—C10—C5	118.0 (3)	C59—C60—C55	117.9 (3)
C7—C11—H11A	109.5	C57—C61—H61A	109.5
C7—C11—H11B	109.5	C57—C61—H61B	109.5
H11A—C11—H11B	109.5	H61A—C61—H61B	109.5
C7—C11—H11C	109.5	C57—C61—H61C	109.5
H11A—C11—H11C	109.5	H61A—C61—H61C	109.5
H11B—C11—H11C	109.5	H61B—C61—H61C	109.5
C17—C12—C13	119.8 (3)	C67—C62—C63	120.2 (4)
C17—C12—C2A	118.0 (3)	C67—C62—C52A	115.0 (4)
C13—C12—C2A	122.2 (3)	C63—C62—C52A	124.7 (4)
C17—C12—C2B	142.1 (4)	C67—C62—C52B	148.8 (5)

C13—C12—C2B	91.7 (4)	C63—C62—C52B	90.1 (5)
C14—C13—C12	119.6 (3)	C64—C63—C62	119.6 (4)
C14—C13—H13	120.2	C64—C63—H63	120.2
C12—C13—H13	120.2	C62—C63—H63	120.2
C13—C14—C15	120.3 (4)	C63—C64—C65	118.8 (4)
C13—C14—H14	119.9	C63—C64—H64	120.6
C15—C14—H14	119.9	C65—C64—H64	120.6
C16—C15—C14	120.0 (4)	C64—C65—C66	121.3 (4)
C16—C15—H15	120.0	C64—C65—H65	119.4
C14—C15—H15	120.0	C66—C65—H65	119.4
C17—C16—C15	119.7 (4)	C67—C66—C65	120.4 (4)
C17—C16—H16	120.1	C67—C66—H66	119.8
C15—C16—H16	120.1	C65—C66—H66	119.8
C16—C17—C12	120.7 (3)	C66—C67—C62	119.7 (4)
C16—C17—H17	119.7	C66—C67—H67	120.2
C12—C17—H17	119.7	C62—C67—H67	120.2

C10—O1—C2A—C3	−48.0 (4)	C60—O51—C52A—C53	−53.5 (4)
C10—O1—C2A—C12	−172.5 (3)	C60—O51—C52A—C62	−178.1 (3)
C10—O1—C2B—C3	29.4 (8)	C60—O51—C52B—C53	24.6 (8)
C10—O1—C2B—C12	154.2 (4)	C60—O51—C52B—C62	150.2 (4)
O1—C2B—C3—C4	−16.9 (8)	O51—C52B—C53—C54	−24.5 (8)
C12—C2B—C3—C4	−138.6 (5)	C62—C52B—C53—C54	−146.5 (5)
O1—C2A—C3—C4	59.1 (4)	O51—C52A—C53—C54	53.7 (5)
C12—C2A—C3—C4	−179.4 (3)	C62—C52A—C53—C54	174.8 (4)
C2B—C3—C4—O4	−178.4 (5)	C52B—C53—C54—O54	−163.3 (5)
C2A—C3—C4—O4	143.3 (4)	C52A—C53—C54—O54	156.3 (4)
C2B—C3—C4—C5	−0.3 (6)	C52B—C53—C54—C55	15.2 (7)
C2A—C3—C4—C5	−38.6 (5)	C52A—C53—C54—C55	−25.3 (5)
O4—C4—C5—C6	7.3 (5)	O54—C54—C55—C56	−3.7 (6)
C3—C4—C5—C6	−170.7 (3)	C53—C54—C55—C56	177.9 (4)
O4—C4—C5—C10	−174.5 (3)	O54—C54—C55—C60	174.8 (4)
C3—C4—C5—C10	7.5 (5)	C53—C54—C55—C60	−3.7 (5)
C10—C5—C6—C7	−0.2 (5)	C60—C55—C56—C57	−0.8 (5)
C4—C5—C6—C7	178.0 (3)	C54—C55—C56—C57	177.6 (3)
C5—C6—C7—C8	−0.4 (5)	C55—C56—C57—C58	−1.6 (5)
C5—C6—C7—C11	179.8 (3)	C55—C56—C57—C61	177.4 (3)
C6—C7—C8—C9	−0.3 (5)	C56—C57—C58—C59	2.0 (5)
C11—C7—C8—C9	179.5 (3)	C61—C57—C58—C59	−177.0 (3)
C7—C8—C9—C10	1.5 (5)	C57—C58—C59—C60	0.0 (5)
C7—C8—C9—Br1	179.5 (3)	C57—C58—C59—Br51	179.9 (3)
C2A—O1—C10—C9	−161.9 (3)	C52B—O51—C60—C59	164.2 (5)
C2B—O1—C10—C9	155.8 (5)	C52A—O51—C60—C59	−155.1 (3)
C2A—O1—C10—C5	16.6 (4)	C52B—O51—C60—C55	−15.7 (6)
C2B—O1—C10—C5	−25.6 (6)	C52A—O51—C60—C55	25.1 (4)
C8—C9—C10—O1	176.6 (3)	C58—C59—C60—O51	177.8 (3)
Br1—C9—C10—O1	−1.4 (4)	Br51—C59—C60—O51	−2.2 (4)
C8—C9—C10—C5	−2.1 (5)	C58—C59—C60—C55	−2.3 (5)

Br1—C9—C10—C5	179.9 (2)	Br51—C59—C60—C55	177.7 (2)
C6—C5—C10—O1	−177.1 (3)	C56—C55—C60—O51	−177.4 (3)
C4—C5—C10—O1	4.7 (5)	C54—C55—C60—O51	4.2 (5)
C6—C5—C10—C9	1.4 (5)	C56—C55—C60—C59	2.7 (5)
C4—C5—C10—C9	−176.8 (3)	C54—C55—C60—C59	−175.7 (3)
O1—C2A—C12—C17	−155.4 (3)	O51—C52A—C62—C67	−128.6 (4)
C3—C2A—C12—C17	82.1 (4)	C53—C52A—C62—C67	108.4 (5)
O1—C2A—C12—C13	26.4 (5)	O51—C52A—C62—C63	52.8 (5)
C3—C2A—C12—C13	−96.1 (4)	C53—C52A—C62—C63	−70.2 (5)
O1—C2B—C12—C17	−124.3 (6)	O51—C52B—C62—C67	−85.1 (9)
C3—C2B—C12—C17	−1.5 (10)	C53—C52B—C62—C67	39.3 (11)
O1—C2B—C12—C13	87.7 (6)	O51—C52B—C62—C63	107.7 (5)
C3—C2B—C12—C13	−149.4 (6)	C53—C52B—C62—C63	−127.9 (6)
C17—C12—C13—C14	0.2 (5)	C67—C62—C63—C64	0.1 (6)
C2A—C12—C13—C14	178.4 (3)	C52A—C62—C63—C64	178.5 (4)
C2B—C12—C13—C14	158.1 (4)	C52B—C62—C63—C64	172.5 (4)
C12—C13—C14—C15	−0.5 (6)	C62—C63—C64—C65	−0.6 (6)
C13—C14—C15—C16	0.1 (6)	C63—C64—C65—C66	0.4 (6)
C14—C15—C16—C17	0.6 (6)	C64—C65—C66—C67	0.5 (7)
C15—C16—C17—C12	−1.0 (6)	C65—C66—C67—C62	−1.1 (7)
C13—C12—C17—C16	0.6 (5)	C63—C62—C67—C66	0.8 (7)
C2A—C12—C17—C16	−177.7 (3)	C52A—C62—C67—C66	−177.8 (4)
C2B—C12—C17—C16	−141.8 (7)	C52B—C62—C67—C66	−164.4 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2*A*—H2*A*···O54^{i}	1.00	2.57	3.396 (5)	140
C53—H53*A*···O4^{ii}	0.99	2.53	3.399 (5)	147

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*, *y*−1, *z*.

(2*E*)-1-(2-Hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (CH2)

Crystal data

$C_{16}H_{14}O_3$
M_r = 254.29
Orthorhombic, $Pca2_1$
a = 25.297 (2) Å
b = 4.0469 (2) Å
c = 12.6390 (16) Å
V = 1293.9 (2) Å^3
Z = 4
F(000) = 536
D_x = 1.305 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3822 reflections
θ = 2.9–34.8°
μ = 0.09 mm^{-1}
T = 100 K
Prism, colourless
0.40 × 0.18 × 0.08 mm

Data collection

Rigaku Xcalibur with a Sapphire3 detector diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0328 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.876, T_{max} = 1.000
12934 measured reflections

3120 independent reflections
3037 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 28.0°$, $\theta_{min} = 3.2°$
$h = -33 \rightarrow 33$
$k = -5 \rightarrow 3$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.078$
$S = 1.05$
3120 reflections
174 parameters
1 restraint
Primary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.1568P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Absolute structure: Flack *x* determined using 1419 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.4 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray data of five flavanone derivatives (**FL1**, **FL2**, **FL3**, **FL5** and **FL8**) were collected on a micro-focus SuperNova diffractometer with an Atlas detector, whereas data collection of two chalcone derivatives (**CH2** and **CH4**) was carried out on an Xcalibur diffractometer with a Sapphire3 detector; all using Mo *Kα* and *ω* scans at a low temperature of 100.0 (1) K. The X-ray data were corrected for absorption using *CrysAlis PRO* (Agilent, 2015). All structures were solved using SHELXT (Sheldrick, 2015a) and refined with SHELXL2014/7 (Sheldrick, 2015b). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.45856 (4)	0.2351 (3)	0.75652 (9)	0.0193 (2)
C6	0.75837 (6)	0.9372 (4)	1.07608 (12)	0.0139 (3)
O2	0.70171 (4)	0.6401 (3)	1.19355 (9)	0.0205 (3)
C10	0.58134 (6)	0.4571 (4)	0.96645 (11)	0.0145 (3)
C8	0.66886 (6)	0.7043 (4)	1.01849 (12)	0.0161 (3)
H8	0.6743	0.7902	0.9511	0.019*
C7	0.70889 (6)	0.7551 (4)	1.10186 (13)	0.0150 (3)
C11	0.58327 (6)	0.5443 (4)	0.85734 (13)	0.0165 (3)
H11	0.6128	0.6532	0.8307	0.020*
C5	0.76789 (6)	1.0843 (4)	0.97529 (12)	0.0159 (3)
H5	0.7418	1.0724	0.9236	0.019*
C9	0.62419 (6)	0.5320 (4)	1.04038 (13)	0.0159 (3)
H9	0.6204	0.4538	1.1092	0.019*
C1	0.79841 (6)	0.9596 (4)	1.15428 (12)	0.0165 (3)
O1	0.79241 (5)	0.8278 (3)	1.25304 (9)	0.0217 (3)
H1	0.7631	0.7420	1.2578	0.033*
C15	0.53645 (6)	0.2906 (4)	1.00442 (13)	0.0166 (3)
H15	0.5348	0.2309	1.0754	0.020*

C16	0.41216 (6)	0.0671 (4)	0.79472 (14)	0.0190 (3)
H16A	0.4220	−0.1450	0.8225	0.029*
H16B	0.3876	0.0381	0.7376	0.029*
H16C	0.3960	0.1961	0.8496	0.029*
C12	0.54173 (6)	0.4687 (4)	0.79068 (12)	0.0170 (3)
H12	0.5432	0.5285	0.7197	0.020*
C13	0.49699 (6)	0.3008 (4)	0.83009 (12)	0.0151 (3)
C14	0.49415 (6)	0.2126 (4)	0.93768 (13)	0.0163 (3)
H14	0.4645	0.1040	0.9640	0.020*
C2	0.84627 (6)	1.1201 (4)	1.13051 (13)	0.0189 (3)
H2	0.8727	1.1331	1.1815	0.023*
C3	0.85432 (6)	1.2604 (4)	1.03064 (14)	0.0190 (3)
H3	0.8862	1.3655	1.0160	0.023*
C4	0.81513 (6)	1.2451 (4)	0.95223 (13)	0.0178 (3)
H4	0.8206	1.3405	0.8862	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0134 (5)	0.0272 (6)	0.0172 (5)	−0.0016 (4)	−0.0022 (4)	−0.0004 (5)
C6	0.0116 (6)	0.0172 (6)	0.0129 (6)	0.0020 (5)	0.0001 (5)	−0.0030 (5)
O2	0.0161 (5)	0.0311 (6)	0.0144 (5)	−0.0010 (5)	0.0000 (4)	0.0023 (5)
C10	0.0124 (6)	0.0159 (6)	0.0152 (7)	0.0013 (5)	0.0001 (5)	−0.0015 (5)
C8	0.0140 (7)	0.0206 (7)	0.0138 (7)	0.0009 (5)	−0.0010 (5)	−0.0008 (6)
C7	0.0127 (6)	0.0184 (7)	0.0141 (7)	0.0019 (5)	0.0011 (5)	−0.0022 (5)
C11	0.0136 (6)	0.0190 (7)	0.0170 (7)	−0.0007 (5)	0.0026 (5)	0.0006 (6)
C5	0.0145 (6)	0.0183 (7)	0.0149 (7)	0.0017 (5)	−0.0008 (5)	−0.0017 (6)
C9	0.0152 (7)	0.0181 (7)	0.0144 (6)	0.0015 (5)	−0.0003 (5)	−0.0002 (6)
C1	0.0163 (7)	0.0203 (7)	0.0127 (7)	0.0028 (5)	−0.0002 (5)	−0.0033 (6)
O1	0.0175 (5)	0.0346 (6)	0.0129 (5)	−0.0027 (5)	−0.0024 (4)	0.0004 (5)
C15	0.0164 (7)	0.0194 (7)	0.0141 (7)	0.0001 (5)	0.0008 (6)	0.0009 (6)
C16	0.0128 (6)	0.0213 (7)	0.0229 (8)	−0.0009 (6)	−0.0019 (5)	−0.0018 (6)
C12	0.0149 (7)	0.0221 (7)	0.0140 (7)	0.0020 (5)	0.0007 (5)	0.0017 (6)
C13	0.0126 (6)	0.0159 (6)	0.0167 (7)	0.0018 (5)	−0.0008 (5)	−0.0022 (6)
C14	0.0134 (6)	0.0187 (6)	0.0170 (7)	−0.0005 (5)	0.0009 (6)	−0.0002 (6)
C2	0.0155 (7)	0.0230 (8)	0.0183 (8)	−0.0002 (6)	−0.0039 (5)	−0.0049 (6)
C3	0.0146 (7)	0.0192 (7)	0.0233 (8)	−0.0015 (5)	0.0019 (6)	−0.0029 (6)
C4	0.0178 (7)	0.0185 (7)	0.0172 (7)	0.0005 (5)	0.0023 (6)	0.0006 (6)

Geometric parameters (Å, º)

O3—C13	1.3712 (18)	C1—O1	1.3659 (19)
O3—C16	1.4399 (19)	C1—C2	1.406 (2)
C6—C1	1.418 (2)	O1—H1	0.8200
C6—C5	1.427 (2)	C15—C14	1.399 (2)
C6—C7	1.489 (2)	C15—H15	0.9300
O2—C7	1.262 (2)	C16—H16A	0.9600
C10—C15	1.405 (2)	C16—H16B	0.9600

C10—C11	1.424 (2)	C16—H16C	0.9600
C10—C9	1.463 (2)	C12—C13	1.411 (2)
C8—C9	1.356 (2)	C12—H12	0.9300
C8—C7	1.476 (2)	C13—C14	1.408 (2)
C8—H8	0.9300	C14—H14	0.9300
C11—C12	1.381 (2)	C2—C3	1.399 (2)
C11—H11	0.9300	C2—H2	0.9300
C5—C4	1.391 (2)	C3—C4	1.403 (2)
C5—H5	0.9300	C3—H3	0.9300
C9—H9	0.9300	C4—H4	0.9300

C13—O3—C16	116.24 (12)	C14—C15—H15	119.3
C1—C6—C5	118.37 (13)	C10—C15—H15	119.3
C1—C6—C7	118.66 (14)	O3—C16—H16A	109.5
C5—C6—C7	122.95 (13)	O3—C16—H16B	109.5
C15—C10—C11	118.51 (14)	H16A—C16—H16B	109.5
C15—C10—C9	118.69 (13)	O3—C16—H16C	109.5
C11—C10—C9	122.80 (13)	H16A—C16—H16C	109.5
C9—C8—C7	119.85 (14)	H16B—C16—H16C	109.5
C9—C8—H8	120.1	C11—C12—C13	120.11 (14)
C7—C8—H8	120.1	C11—C12—H12	119.9
O2—C7—C8	120.36 (13)	C13—C12—H12	119.9
O2—C7—C6	120.31 (14)	O3—C13—C14	124.73 (13)
C8—C7—C6	119.32 (14)	O3—C13—C12	115.00 (13)
C12—C11—C10	120.63 (14)	C14—C13—C12	120.26 (14)
C12—C11—H11	119.7	C15—C14—C13	119.10 (14)
C10—C11—H11	119.7	C15—C14—H14	120.4
C4—C5—C6	121.80 (14)	C13—C14—H14	120.4
C4—C5—H5	119.1	C3—C2—C1	120.37 (14)
C6—C5—H5	119.1	C3—C2—H2	119.8
C8—C9—C10	126.41 (14)	C1—C2—H2	119.8
C8—C9—H9	116.8	C2—C3—C4	121.09 (14)
C10—C9—H9	116.8	C2—C3—H3	119.5
O1—C1—C2	118.12 (13)	C4—C3—H3	119.5
O1—C1—C6	122.18 (14)	C5—C4—C3	118.65 (14)
C2—C1—C6	119.70 (14)	C5—C4—H4	120.7
C1—O1—H1	109.5	C3—C4—H4	120.7
C14—C15—C10	121.38 (14)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	1.80	2.532 (2)	147
C5—H5···O1^{i}	0.93	2.53	3.364 (5)	150
C9—H9···O2	0.93	2.44	2.790 (2)	103

Symmetry code: (i) −*x*+3/2, *y*, *z*−1/2.

(2*E*)-1-(2-Hydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one (CH4)

Crystal data

$C_{15}H_{12}O_3$
$M_r = 240.26$
Monoclinic, $P2_1$
$a = 3.9413$ (2) Å
$b = 17.3664$ (8) Å
$c = 17.2360$ (9) Å
$\beta = 94.504$ (5)°
$V = 1176.10$ (10) Å^3
$Z = 4$
$F(000) = 504$
$D_x = 1.357$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4020 reflections
$\theta = 3.1$–$30.3°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Needle, light yellow
0.50 × 0.08 × 0.06 mm

Data collection

Rigaku Xcalibur with a Sapphire3 detector diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0328 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
$T_{min} = 0.758$, $T_{max} = 1.000$
9466 measured reflections
4835 independent reflections
4459 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 26.5°$, $\theta_{min} = 3.3°$
$h = -4 \rightarrow 2$
$k = -21 \rightarrow 21$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.073$
$S = 1.04$
4835 reflections
329 parameters
1 restraint
Primary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 0.027P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Absolute structure: Flack *x* determined using 1981 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.2 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray data of five flavanone derivatives (**FL1**, **FL2**, **FL3**, **FL5** and **FL8**) were collected on a micro-focus SuperNova diffractometer with an Atlas detector, whereas data collection of two chalcone derivatives (**CH2** and **CH4**) was carried out on an Xcalibur diffractometer with a Sapphire3 detector; all using Mo $K\alpha$ and ω scans at a low temperature of 100.0 (1) K. The X-ray data were corrected for absorption using *CrysAlis PRO* (Agilent, 2015). All structures were solved using SHELXT (Sheldrick, 2015a) and refined with SHELXL2014/7 (Sheldrick, 2015b). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C13	0.9411 (5)	0.03886 (12)	0.03812 (12)	0.0169 (4)

O3	0.9956 (4)	−0.03834 (9)	0.02569 (9)	0.0227 (4)
H31	1.0911	−0.0439	−0.0145	0.034*
C15	0.9684 (5)	0.17217 (12)	0.00239 (13)	0.0176 (4)
H15	1.0222	0.2098	−0.0331	0.021*
C7	0.5989 (5)	0.38907 (13)	0.16070 (12)	0.0161 (4)
O1	0.3998 (4)	0.54764 (8)	0.17933 (9)	0.0229 (4)
H1	0.4938	0.5262	0.1444	0.034*
C1	0.3565 (5)	0.49670 (12)	0.23710 (12)	0.0166 (4)
C11	0.7536 (5)	0.13645 (13)	0.12486 (13)	0.0177 (4)
H11	0.6654	0.1498	0.1715	0.021*
O2	0.6684 (4)	0.43589 (9)	0.10800 (9)	0.0211 (3)
C14	1.0210 (5)	0.09514 (12)	−0.01494 (12)	0.0170 (4)
H14	1.1088	0.0814	−0.0615	0.020*
C9	0.7817 (5)	0.27615 (12)	0.08745 (12)	0.0168 (4)
H9	0.8397	0.3106	0.0493	0.020*
C2	0.2079 (5)	0.52406 (12)	0.30296 (13)	0.0195 (5)
H2	0.1403	0.5753	0.3053	0.023*
C12	0.8031 (5)	0.05960 (13)	0.10760 (12)	0.0183 (4)
H12	0.7445	0.0217	0.1422	0.022*
C6	0.4512 (5)	0.41799 (12)	0.23158 (12)	0.0149 (4)
C5	0.4013 (5)	0.37025 (13)	0.29599 (13)	0.0188 (5)
H5	0.4639	0.3187	0.2942	0.023*
C10	0.8353 (5)	0.19456 (12)	0.07252 (12)	0.0154 (4)
C3	0.1617 (5)	0.47520 (13)	0.36434 (13)	0.0200 (5)
H3	0.0629	0.4938	0.4079	0.024*
C8	0.6555 (5)	0.30652 (13)	0.15150 (12)	0.0174 (4)
H8	0.6027	0.2735	0.1913	0.021*
C4	0.2616 (5)	0.39798 (13)	0.36184 (13)	0.0212 (5)
H4	0.2346	0.3656	0.4039	0.025*
C57	0.1018 (5)	0.18931 (13)	0.47758 (13)	0.0184 (4)
O52	−0.0700 (4)	0.24253 (9)	0.44346 (9)	0.0242 (4)
C54	0.5135 (5)	0.00057 (14)	0.42175 (14)	0.0225 (5)
H54	0.6135	−0.0428	0.4456	0.027*
C52	0.3281 (6)	0.07091 (14)	0.30441 (13)	0.0231 (5)
H52	0.3078	0.0742	0.2504	0.028*
C59	0.0571 (5)	0.25093 (13)	0.60366 (13)	0.0188 (4)
H59	−0.0806	0.2858	0.5749	0.023*
C58	0.1765 (5)	0.19171 (13)	0.56340 (13)	0.0189 (4)
H58	0.3038	0.1529	0.5889	0.023*
C55	0.3911 (5)	0.05940 (13)	0.46626 (13)	0.0197 (5)
H55	0.4130	0.0553	0.5202	0.024*
C53	0.4848 (5)	0.00718 (14)	0.34053 (13)	0.0233 (5)
H53	0.5715	−0.0315	0.3104	0.028*
O51	0.0512 (4)	0.19141 (10)	0.31041 (9)	0.0274 (4)
H51	−0.0333	0.2199	0.3416	0.041*
C56	0.2333 (5)	0.12558 (13)	0.43147 (13)	0.0184 (4)
C51	0.2006 (5)	0.13030 (13)	0.34893 (13)	0.0201 (5)
C60	0.1163 (5)	0.26743 (12)	0.68702 (13)	0.0183 (4)

O53	0.3185 (4)	0.32903 (9)	0.92116 (9)	0.0242 (4)
H531	0.2297	0.3703	0.9308	0.036*
C62	0.3580 (5)	0.23908 (13)	0.81908 (13)	0.0197 (4)
H62	0.4764	0.2060	0.8540	0.024*
C64	0.0487 (5)	0.35869 (13)	0.79190 (13)	0.0202 (5)
H64	−0.0381	0.4049	0.8090	0.024*
C65	−0.0099 (5)	0.33729 (13)	0.71422 (13)	0.0197 (4)
H65	−0.1346	0.3697	0.6798	0.024*
C61	0.2975 (5)	0.21824 (13)	0.74172 (13)	0.0191 (5)
H61	0.3770	0.1711	0.7252	0.023*
C63	0.2396 (5)	0.31046 (13)	0.84470 (12)	0.0186 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C13	0.0187 (10)	0.0134 (10)	0.0183 (10)	0.0007 (8)	0.0002 (8)	−0.0032 (8)
O3	0.0352 (9)	0.0136 (8)	0.0207 (8)	0.0014 (7)	0.0107 (7)	−0.0011 (7)
C15	0.0210 (10)	0.0159 (11)	0.0161 (10)	0.0000 (9)	0.0024 (8)	0.0014 (8)
C7	0.0157 (10)	0.0163 (10)	0.0159 (10)	−0.0021 (8)	−0.0017 (8)	−0.0006 (9)
O1	0.0341 (9)	0.0136 (8)	0.0217 (8)	0.0021 (7)	0.0056 (7)	0.0014 (7)
C1	0.0158 (10)	0.0154 (10)	0.0180 (10)	−0.0020 (9)	−0.0015 (8)	−0.0002 (9)
C11	0.0225 (10)	0.0175 (11)	0.0133 (10)	0.0006 (9)	0.0042 (8)	−0.0019 (8)
O2	0.0305 (8)	0.0152 (7)	0.0183 (7)	−0.0003 (7)	0.0065 (6)	0.0008 (6)
C14	0.0215 (11)	0.0176 (11)	0.0120 (10)	0.0022 (9)	0.0029 (8)	−0.0008 (8)
C9	0.0166 (10)	0.0153 (10)	0.0184 (10)	−0.0018 (8)	0.0007 (8)	0.0026 (8)
C2	0.0189 (10)	0.0143 (10)	0.0250 (11)	0.0005 (9)	0.0008 (9)	−0.0044 (9)
C12	0.0244 (10)	0.0162 (11)	0.0146 (10)	−0.0010 (9)	0.0033 (8)	0.0036 (8)
C6	0.0138 (9)	0.0149 (10)	0.0158 (10)	−0.0013 (8)	−0.0005 (8)	−0.0020 (8)
C5	0.0201 (10)	0.0145 (11)	0.0218 (11)	−0.0008 (9)	0.0014 (9)	−0.0002 (8)
C10	0.0149 (9)	0.0152 (10)	0.0160 (10)	−0.0017 (8)	0.0005 (8)	−0.0006 (8)
C3	0.0177 (10)	0.0230 (12)	0.0198 (11)	−0.0042 (9)	0.0036 (9)	−0.0080 (9)
C8	0.0223 (11)	0.0134 (10)	0.0166 (10)	0.0009 (9)	0.0026 (8)	0.0014 (9)
C4	0.0241 (11)	0.0223 (12)	0.0176 (10)	−0.0048 (10)	0.0042 (9)	0.0012 (9)
C57	0.0156 (9)	0.0177 (11)	0.0217 (11)	−0.0045 (9)	0.0009 (8)	0.0009 (9)
O52	0.0300 (8)	0.0182 (8)	0.0239 (8)	0.0022 (7)	−0.0003 (7)	0.0030 (7)
C54	0.0191 (10)	0.0177 (11)	0.0307 (12)	−0.0002 (9)	0.0024 (9)	−0.0002 (10)
C52	0.0248 (11)	0.0262 (12)	0.0189 (11)	−0.0099 (10)	0.0055 (9)	−0.0017 (9)
C59	0.0162 (10)	0.0172 (11)	0.0230 (11)	−0.0007 (9)	0.0016 (8)	0.0009 (9)
C58	0.0180 (10)	0.0180 (11)	0.0206 (10)	0.0004 (9)	0.0017 (8)	0.0025 (9)
C55	0.0171 (10)	0.0217 (12)	0.0205 (11)	−0.0031 (9)	0.0020 (8)	0.0028 (9)
C53	0.0188 (10)	0.0225 (12)	0.0294 (12)	−0.0060 (9)	0.0080 (9)	−0.0073 (10)
O51	0.0410 (9)	0.0205 (8)	0.0202 (8)	−0.0006 (7)	−0.0009 (7)	0.0023 (7)
C56	0.0166 (9)	0.0180 (11)	0.0204 (11)	−0.0051 (9)	0.0012 (8)	−0.0008 (9)
C51	0.0213 (10)	0.0178 (11)	0.0210 (11)	−0.0079 (9)	0.0008 (9)	0.0024 (9)
C60	0.0148 (9)	0.0171 (11)	0.0238 (11)	−0.0012 (9)	0.0055 (8)	−0.0005 (9)
O53	0.0371 (9)	0.0157 (8)	0.0203 (8)	0.0013 (7)	0.0048 (7)	−0.0019 (6)
C62	0.0200 (10)	0.0150 (11)	0.0247 (11)	0.0000 (9)	0.0051 (9)	0.0027 (9)
C64	0.0203 (11)	0.0126 (10)	0.0288 (12)	−0.0007 (8)	0.0073 (9)	−0.0002 (9)

C65	0.0172 (10)	0.0169 (11)	0.0252 (11)	0.0004 (9)	0.0032 (9)	0.0036 (9)
C61	0.0183 (10)	0.0134 (10)	0.0263 (11)	−0.0003 (8)	0.0058 (9)	−0.0023 (9)
C63	0.0212 (10)	0.0153 (10)	0.0200 (11)	−0.0051 (9)	0.0062 (9)	−0.0007 (9)

Geometric parameters (Å, º)

C13—O3	1.377 (3)	C57—O52	1.263 (3)
C13—C14	1.391 (3)	C57—C56	1.480 (3)
C13—C12	1.401 (3)	C57—C58	1.486 (3)
O3—H31	0.8200	C54—C55	1.387 (3)
C15—C14	1.390 (3)	C54—C53	1.400 (3)
C15—C10	1.410 (3)	C54—H54	0.9300
C15—H15	0.9300	C52—C53	1.390 (3)
C7—O2	1.265 (3)	C52—C51	1.402 (3)
C7—C8	1.462 (3)	C52—H52	0.9300
C7—C6	1.482 (3)	C59—C58	1.346 (3)
O1—C1	1.353 (3)	C59—C60	1.466 (3)
O1—H1	0.8200	C59—H59	0.9300
C1—C2	1.401 (3)	C58—H58	0.9300
C1—C6	1.422 (3)	C55—C56	1.417 (3)
C11—C12	1.385 (3)	C55—H55	0.9300
C11—C10	1.408 (3)	C53—H53	0.9300
C11—H11	0.9300	O51—C51	1.361 (3)
C14—H14	0.9300	O51—H51	0.8200
C9—C8	1.353 (3)	C56—C51	1.421 (3)
C9—C10	1.458 (3)	C60—C65	1.406 (3)
C9—H9	0.9300	C60—C61	1.422 (3)
C2—C3	1.379 (3)	O53—C63	1.368 (3)
C2—H2	0.9300	O53—H531	0.8200
C12—H12	0.9300	C62—C61	1.384 (3)
C6—C5	1.412 (3)	C62—C63	1.408 (3)
C5—C4	1.386 (3)	C62—H62	0.9300
C5—H5	0.9300	C64—C65	1.391 (3)
C3—C4	1.399 (3)	C64—C63	1.410 (3)
C3—H3	0.9300	C64—H64	0.9300
C8—H8	0.9300	C65—H65	0.9300
C4—H4	0.9300	C61—H61	0.9300
O3—C13—C14	122.38 (19)	O52—C57—C56	119.64 (19)
O3—C13—C12	117.33 (19)	O52—C57—C58	120.0 (2)
C14—C13—C12	120.29 (19)	C56—C57—C58	120.35 (19)
C13—O3—H31	109.5	C55—C54—C53	119.2 (2)
C14—C15—C10	121.4 (2)	C55—C54—H54	120.4
C14—C15—H15	119.3	C53—C54—H54	120.4
C10—C15—H15	119.3	C53—C52—C51	120.4 (2)
O2—C7—C8	120.60 (18)	C53—C52—H52	119.8
O2—C7—C6	119.70 (19)	C51—C52—H52	119.8
C8—C7—C6	119.68 (18)	C58—C59—C60	128.3 (2)

C1—O1—H1	109.5	C58—C59—H59	115.9
O1—C1—C2	117.37 (19)	C60—C59—H59	115.9
O1—C1—C6	122.03 (19)	C59—C58—C57	119.0 (2)
C2—C1—C6	120.59 (19)	C59—C58—H58	120.5
C12—C11—C10	120.67 (19)	C57—C58—H58	120.5
C12—C11—H11	119.7	C54—C55—C56	121.6 (2)
C10—C11—H11	119.7	C54—C55—H55	119.2
C15—C14—C13	119.31 (19)	C56—C55—H55	119.2
C15—C14—H14	120.3	C52—C53—C54	120.7 (2)
C13—C14—H14	120.3	C52—C53—H53	119.6
C8—C9—C10	126.2 (2)	C54—C53—H53	119.6
C8—C9—H9	116.9	C51—O51—H51	109.5
C10—C9—H9	116.9	C55—C56—C51	118.2 (2)
C3—C2—C1	120.1 (2)	C55—C56—C57	122.7 (2)
C3—C2—H2	119.9	C51—C56—C57	119.12 (19)
C1—C2—H2	119.9	O51—C51—C52	117.8 (2)
C11—C12—C13	120.2 (2)	O51—C51—C56	122.4 (2)
C11—C12—H12	119.9	C52—C51—C56	119.8 (2)
C13—C12—H12	119.9	C65—C60—C61	118.0 (2)
C5—C6—C1	117.28 (19)	C65—C60—C59	117.54 (19)
C5—C6—C7	122.51 (19)	C61—C60—C59	124.44 (19)
C1—C6—C7	120.20 (18)	C63—O53—H531	109.5
C4—C5—C6	121.9 (2)	C61—C62—C63	119.7 (2)
C4—C5—H5	119.0	C61—C62—H62	120.1
C6—C5—H5	119.0	C63—C62—H62	120.1
C11—C10—C15	118.11 (19)	C65—C64—C63	120.2 (2)
C11—C10—C9	122.66 (19)	C65—C64—H64	119.9
C15—C10—C9	119.22 (19)	C63—C64—H64	119.9
C2—C3—C4	120.8 (2)	C64—C65—C60	121.0 (2)
C2—C3—H3	119.6	C64—C65—H65	119.5
C4—C3—H3	119.6	C60—C65—H65	119.5
C9—C8—C7	122.68 (19)	C62—C61—C60	121.4 (2)
C9—C8—H8	118.7	C62—C61—H61	119.3
C7—C8—H8	118.7	C60—C61—H61	119.3
C5—C4—C3	119.3 (2)	O53—C63—C62	116.98 (19)
C5—C4—H4	120.4	O53—C63—C64	123.43 (19)
C3—C4—H4	120.4	C62—C63—C64	119.6 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	1.84	2.570 (2)	147
O3—H31···O2^{i}	0.82	1.96	2.783 (5)	176
O51—H51···O52	0.82	1.82	2.539 (2)	146
O53—H531···O3^{ii}	0.82	1.99	2.803 (2)	169

C4—H4···O52	0.93	2.57	3.356 (3)	143
C15—H15···O53^{iii}	0.93	2.53	3.404 (3)	156

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*; (ii) −*x*+1, *y*+1/2, −*z*+1; (iii) *x*+1, *y*, *z*−1.